

ANALYTIC AND NUMERICAL TRANSPORT TECHNIQUES IN
ENERGY-DEPENDENT FAST NEUTRON WAVE
AND PULSE PROPAGATION

By

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Abstract of Dissertation Presented to the
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ANALYTIC AND NUMERICAL TRANSPORT TECHNIQUES IN ENERGY-DEPENDENT
FAST NEUTRON WAVE AND PULSE PROPAGATION

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Neutron wave and pulse propagation analysis is a natural approach to space-dependent kinetics in subprompt critical media. Prior to the present work, analytic treatments of fast media have been few and limited in scope, in contrast to thermal wave and pulse propagation, which has been studied rather thoroughly and with quite sophisticated techniques.

The principal difference between analysis of fast and thermal systems is treating the slowing-down operator. A formal approach is presented for arbitrary slowing-down operators; the spectrum, eigenfunctions, and adjoint eigenfunctions of the slab-geometry energy-dependent wave transport operator are obtained, using the singular eigenfunction technique. Both multiplying and nonmultiplying media are treated. Fission is modeled by a one-term separable kernel, although

the extension to a multiterm degenerate fission kernel, representing several fissionable species, is apparent.

The fast neutron wave singular eigenfunction results are compared with other energy-dependent transport work, particularly with previous thermal eigenfunction analysis, and with work on static fast neutron transport using an energy transform approach. Wave transport in fast multiplying media and in thermal noncrystalline media (modeled by a separable thermalization kernel) are rather similar in that due to energy-regenerative interaction processes a discrete asymptotic separable eigenmode exists for moderate values of wave frequency and absorption cross sections. The dispersion laws obeyed by the eigenvalues associated with these modes are qualitatively quite comparable. The fast nonmultiplying case has no direct thermal analogue other than the nonphysical "absorption only" model. It is found that the presence of down-scattering in this case gives rise to singular continuum eigenfunctions which are not as simply interpreted as the straightforward streaming modes obtained for zero scattering cross section. Nevertheless, these results appear to be in qualitative agreement with other work on energy-dependent fast neutron transport theory.

The formal analytic results are developed in several directions to investigate their applicability to practical calculations. A major portion of this work is devoted to obtaining the energy-dependent wave transport representation of the transfer matrix method, which provides a formalism for implementing calculations concerning wave and pulse propagation through finite regions such as adjacent slabs of different composition. It is found that, for isotropic scattering, the basic operators

of the transfer matrix formalism can be constructed from eigenfunctions of the wave transport operator. This result is general and is equally applicable to fast and thermal analysis.

Finally, the dispersion law expression for a fast multiplying medium is employed to develop an algorithm for computing the discrete eigenfunctions and associated dispersion law for separable and degenerate fission kernels. A specific application of this method then is made to the case of isotropic elastic and inelastic scattering from any number of nuclides and levels, with arbitrary lethargy dependence of cross sections. Elastic scattering is modeled by a free gas kernel, and inelastic scattering by a constant energy loss per interaction per level. Unlike techniques requiring inversion of matrices, computation time increases approximately linearly with increases in lethargy steps, making quite detailed computations feasible. Illustrative computations are carried out using constant cross sections and a single elastic scattering species.

CHAPTER I

INTRODUCTION

Purpose

As the demand for energy increases and supplies of economically recoverable fuels diminish, fast breeder reactors will supply an increasing proportion of base-load generated power. To operate most economically these reactors will tend to be as large as is technologically feasible. Accordingly, as the size of fast reactor cores increases, it will become increasingly important to understand spatially dependent kinetic effects in fast systems.

A particularly straightforward method of investigating propagation of neutronic disturbances in fast reactor materials is to place a pulsed or oscillating source of neutrons at the face of an experimental assembly, and then to observe the propagation of the neutron "signal" through the assembly. In this way one can study spatially dependent flux oscillations such as might be expected to result from flow-induced vibrations of core components, void formation and collapse, and other such phenomena.

Neutron wave and pulse propagation experiments have been performed in many different thermal media, both multiplying and nonmultiplying. The theoretical basis of analysis of thermal wave propagation in

nonmultiplying media has attained a considerable degree of sophistication, and fairly accurate numerical prediction of some experimental results is possible. This is in contrast to the situation in the fast neutron wave regime; few experiments have been performed, and analytic investigations have been hampered by difficulties which do not arise in treatment of thermal systems. The purpose of this dissertation is to present a particular framework of approach within which these difficulties may be addressed, extending techniques which have been applied primarily to thermal analysis.

Three general objectives will be pursued:

- (i) to develop the spectral representation of the energy-dependent fast wave Boltzmann operator as far as possible in sufficiently general form so that its potential for use with realistic cross section data can be evaluated;
- (ii) to extend a formalism which treats neutron transport in finite and discontinuous media so that the above results may be applied to wave transport in experimentally realistic geometries and through successive regions; and
- (iii) to illustrate applications of the analysis by computing the fundamental eigenfunction and dispersion law for wave propagation in fast multiplying media, using a modelled kernel in the Boltzmann operator.

Early Neutron Wave Investigations

In 1948 Weinberg and Schweinler published the first description in the open literature of the generation and analysis of neutron waves [1].

Using one-speed diffusion theory they were able to show that a localized oscillation in neutron absorption within a reactor would produce a perturbation in the neutron population which would propagate in wave-like fashion. The first experiments with neutron waves were reported in 1955 by Raievski and Horowitz [2], using a mechanically modulated exterior source to generate waves in D_2O and graphite. Uhrig [3] then applied this technique to measurements in subcritical assemblies. Both experimental and theoretical aspects of neutron wave propagation subsequently received considerable attention and refinement, particularly by Perez [4] and his associates at the University of Florida, although experiments and most analytic efforts were restricted to thermal systems.

As investigation of the theoretical basis of neutron wave experiments proceeded, it was realized that from an analytic standpoint experiments involving spatially propagating pulses were equivalent to neutron wave experiments, since any physically realizable pulse could be time-Fourier analyzed to give its frequency components [5]. Also, it became clear that neutron wave propagation was related to other linear static and kinetic experimental techniques, in particular the classical exponential experiment, which is the zero-frequency limit of the wave experiment, and the pulse die-away experiment [5-8]. (The die-away experiment monitors the time-rate of decay of a neutron population which has been introduced into a finite assembly by a pulsed external source. For technical reasons this type of experiment was easier to perform than wave experiments, and enjoyed a more rapid initial development [4].) As a result, these methods experienced

considerable parallel theoretical treatment [8-10]. Early work in this area is reviewed extensively by Uhrig [7] and Perez and Uhrig [4].

Fast Neutron Wave Investigations

Neutron wave and pulse propagation has received proportionately very little attention in the fast energy regime. The only experiments described in the literature, performed by Napolitano et al. [11,12] and Paiano et al. [13] at the University of Florida, have been in nonmultiplying media; no experiments in multiplying media have been reported. The technical difficulty of such experiments probably has contributed both to the lack of experimental data and the scarcity of methods to predict and correlate results. Theoretical analysis also has been retarded by the fact that even tractable energy-dependent analytic models of fast media do not have convenient mathematical properties, and consequently most of the elegant techniques which have been applied to thermal neutron transport cannot be extended readily to this problem [14]. Notable exceptions to the general absence of numerical techniques and results are the multi-group, multiplying medium calculations of Travelli [15,16], and the calculations of Booth et al. [17], using the multi-group discrete ordinates method of Dodds et al. [18] to interpret Napolitano's experimental results.

Energy-Dependent Transport Formulation of Wave and Pulse Propagation

Before discussing the various theoretical results which are directly or indirectly applicable to fast neutron wave and pulse

propagation, it will be helpful to approach the general neutron wave problem from the point of view of the energy-dependent transport method which will be used in this dissertation. We begin with the classic time-dependent Boltzmann equation for the neutron flux [19,20,21], which we will write

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, \vec{\Omega}, t) + \vec{\Omega} \cdot \nabla \phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(E) \phi(\vec{r}, E, \vec{\Omega}, t) - \int_{4\pi} d\vec{\Omega}' \int_0^{\infty} dE' K(E', \vec{\Omega}' \rightarrow E, \Omega) \phi(\vec{r}, E', \vec{\Omega}', t) = S(\vec{r}, E, \Omega, t) \quad (1.1)$$

In standard notation, $\phi(\vec{r}, E, \vec{\Omega}, t)$ is the neutron directional flux, v is the neutron speed, $\vec{\Omega}$ is the unit vector in the direction of neutron travel, E is the neutron energy, \vec{r} is the spatial coordinate, $\Sigma_t(E)$ is the total cross section, and $S(\vec{r}, E, \vec{\Omega}, t)$ is a flux-independent source term. The interaction kernel $K(E', \vec{\Omega}' \rightarrow E, \vec{\Omega})$ contains all neutron interaction processes which give rise to secondary neutrons with altered energy and direction. All cross sections (and thus K) are taken to be region-wise independent of \vec{r} , and the medium described by the equation is assumed to be isotropic in the sense that interaction properties do not depend on the initial direction of neutron travel. Cross sections also are assumed to be constant with respect to time and independent of the flux; neutron wave and pulse propagation experiments meet these two criteria quite well. Propagation of disturbances in sub-prompt critical reactors also should be adequately described by this linear kinetic

model. (Nonlinear space-dependent kinetics are of interest primarily in the context of excursion situations; such problems, while important, are difficult to analyze, and thus far have been approached by use of specialized and involved computational techniques [22,23,24].)

Any of a number of classic analytic approaches can be taken to the solution of Eq. (1.1); here we will treat it as an eigenvalue problem. This will enable us to extend our results to finite medium and multi-region problems; the transfer matrix formalism, which will be discussed in Chapter III, requires solution of a similar eigenvalue equation, and we will be able to relate its solution to those of the wave Boltzmann equation for isotropic scattering. Furthermore, we can make use of spectral analysis which already has been done on the thermal neutron version of Eq. (1.1).

Plane Symmetry and the Eigenvalue Equation

The mathematical development of transport theory has reached its greatest sophistication for the case of plane symmetry, and this is true also for the particular subject of neutron wave and pulse propagation. Since this geometry also is appropriate for the description of classical wave and pulse propagation experiments, we will turn our attention to the specific case of plane neutron waves. The infinite medium plane wave eigenfunctions which will be obtained may then be used in developing the corresponding transfer matrix formalism, which can be employed to study the propagation of waves and pulses through finite slabs and successive slabs of dissimilar materials.

Following customary arguments, we stipulate that all sources or initial fluxes must be rotationally symmetric about the x axis and do not depend on the transverse Cartesian coordinates y and z. Orienting the x axis along the direction of wave propagation, we have for the transport operator of Eq. (1.1)

$$\vec{\Omega} \cdot \Delta = \mu \frac{\partial}{\partial x} ; \quad \mu \equiv \vec{\Omega} \cdot \hat{x} \quad (1.2)$$

where \hat{x} is the unit vector in the x direction, and μ is the cosine of the angle between the path of neutron travel and the x axis. With the restrictions of Eq. (1.2) the homogeneous Boltzmann equation may be written

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t} \phi(x, E, \mu, t) + \mu \frac{\partial}{\partial x} \phi(x, E, \mu, t) + \Sigma_t(E) \phi(x, E, \mu, t) \\ - \int_{-1}^1 d\mu' \int_0^{\infty} dE' K(E', \mu' \rightarrow E, \mu) \phi(x, E', \mu', t) = 0. \end{aligned} \quad (1.3)$$

We notice that time and space operators appear only in the first two terms, respectively, while the integral operator acts on E and μ . Consequently, x and t variables may be separated. With appropriate choices for the separation constants ϕ may be expressed as a damped plane wave

$$\begin{aligned}\phi_{\kappa}(x, E, \mu, t) &= F(E, \mu; \kappa) e^{i\omega t} e^{-\kappa x} \\ &= F(E, \mu; \kappa) e^{-\alpha x} e^{i(\omega t - \xi x)}\end{aligned}\quad (1.4)$$

where ω is the wave or Fourier-component frequency, and κ is a complex constant, $\kappa \equiv \alpha + i\xi$, the complex inverse relaxation length. Thus α is the inverse relaxation length of the wave, while ξ is its wave number. The frequency ω will be regarded as a parameter of the equation, and we will treat κ as the eigenvalue to be determined. Introducing Eq. (1.4) into Eq. (1.3)

$$\left(\frac{i\omega}{v} - \mu\kappa + \Sigma_t(E) \right) F(E, \mu; \kappa) - \int_{-1}^1 d\mu' \int_0^{\infty} dE' K(E', \mu' \rightarrow E, \mu) F(E', \mu'; \kappa) = 0, \quad (1.5)$$

or defining

$$a(E, \omega) \equiv \Sigma_t(E) + \frac{i\omega}{v}(E) \quad (1.6)$$

Eq. (1.5) has the form

$$(a(E, \omega) - \mu\kappa) F(E, \mu; \kappa) - \int_{-1}^1 d\mu' \int_0^{\infty} dE' K(E', \mu' \rightarrow E, \mu) F(E', \mu'; \kappa) = 0 \quad (1.7)$$

which will be referred to as the wave Boltzmann equation, or WBE, throughout the rest of this work. This is the most general statement of the Boltzmann equation in wave eigenvalue form with plane symmetry. As an eigenvalue problem it should more properly be written

$$\int_{-1}^1 d\mu' \int_0^\infty dE' \left(\frac{a(E, \omega)}{\mu} \delta(E-E') \delta(\mu-\mu') - \frac{1}{\mu} K(E', \mu' \rightarrow E, \mu) \right) F(E', \mu'; \kappa) = \kappa F(E, \mu; \kappa). \quad (1.8)$$

The pole at $\mu = 0$ causes no difficulties which we will need to consider [25]; this value of μ corresponds to a direction of neutron travel perpendicular to the direction of wave propagation.

Interaction Operators for the Fast and Thermal Neutron Regimes

The two general types of neutron interaction which are of importance in wave and pulse propagation and which enter into the kernel of Eq. (1.7) are scattering and fission. Adopting for a moment a theoretician's perspective on reality, we may define a fast neutron experiment as one in which the scattering kernel has a Volterra form in energy. In a similar vein a thermal problem may be distinguished by the presence of a Fredholm scattering kernel. These observations stem from the fact that in the fast neutron regime one is concerned with neutron energies from the eV range to about 10 MeV, the upper end of the fission spectrum; hence only downscattering in energy is important. By contrast,

in the thermal regime neutrons are in or near thermal equilibrium with their surroundings so that upscattering in energy occurs as well; energies of interest range essentially over the thermal Maxwellian spectrum.

Appropriate interaction kernel models reflect these properties. We may write the thermal scattering contribution to the interaction kernel as

$$\int_{-1}^1 d\mu' \int_0^{\infty} dE' \Sigma_S(E', \mu' \rightarrow E, \mu) \cdot$$

while the fast scattering operator has the form

$$\int_{-1}^1 d\mu' \int_E^{\infty} dE' \Sigma_S(E', \mu' \rightarrow E, \mu) \cdot$$

extending the notation of Eq.s (1.3) to (1.7).

In multiplying media the interaction kernel contains a contribution due to fission in addition to scattering. Difficulties associated with treating the slowing down of fission neutrons [26] have precluded transport analysis of wave propagation in thermal multiplying media, although other models such as age-diffusion have been employed [27]. No such problem arises in the fast multiplying wave problem, since the energy range of the fission spectrum is essentially the energy range of interest.

For the fission contribution to the interaction operator we will use the customary isotropic separable kernel

$$\chi(E) \nu \Sigma_f(E').$$

When only one fissionable isotope is present this is a satisfactory model. For two or more fissionable species, one can either construct an equivalent separable kernel with averaged χ and $\nu \Sigma_f$ or employ a degenerate kernel

$$\sum_{j=1}^J \chi^{(j)}(E) \nu \Sigma_f^{(j)}(E').$$

Only the separable kernel will be treated in detail here but the formalism of Chapter II can be extended in a straightforward way to degenerate kernels for multiple fissioning species.

To avoid the appearance of unwelcome factors of 1/2 in connection with the isotropic fission spectrum, we will make the following notational distinction. Define the isotropic $\chi(E)$ so that

$$\int_0^{\infty} \chi(E) dE = 1. \quad (1.9)$$

Define χ so that

$$\chi \equiv \chi(E, \mu) = 1/2 \chi(E); \quad (1.10)$$

then

$$\int_{-1}^1 d\mu \int_0^{\infty} dE \chi = 1. \quad (1.11)$$

The fission interaction operator employing the separable kernel model and Eq. (1.10) thus becomes

$$\chi \int_{-1}^1 d\mu' \int_0^{\infty} dE' v\Sigma_f(E').$$

which is the form which will be used throughout this work.

Using the above forms for contributions to the interaction kernel the fast homogeneous WBE of Eq. (1.7) may be written

$$(a - \mu\kappa)F(E, \mu; \kappa) = \int_{-1}^1 d\mu' \int_E^{\infty} dE' \Sigma_S(E', \mu' \rightarrow E, \mu)F(E', \mu'; \kappa) \quad (1.12)$$

for nonmultiplying media, and

$$\begin{aligned} (a - \mu\kappa)F(E, \mu; \kappa) &= \int_{-1}^1 d\mu' \int_E^{\infty} dE' \Sigma_S(E', \mu' \rightarrow E, \mu)F(E', \mu'; \kappa) \\ &+ \chi \int_{-1}^1 d\mu' \int_0^{\infty} dE' v\Sigma_f(E')F(E', \mu'; \kappa) \end{aligned} \quad (1.13)$$

for multiplying media.

It should be noted that we have taken into account only prompt neutrons in Eq (1.13), and hence ν here is the number of prompt neutrons per fission. Delayed neutrons will contribute only at wave periods greater than the shortest delayed neutron precursor lifetime, an effect which has been investigated numerically by Travelli [16]. Also, it will be assumed that the medium under consideration is subprompt critical.

The thermal nonmultiplying WBE, which will be discussed as a point of departure for our work on Eq. (1.13), is

$$(a - \mu\kappa)F(E, \mu; \kappa) = \int_{-1}^1 d\mu' \int_0^{\infty} dE' \Sigma_S(E', \mu' \rightarrow E, \mu)F(E', \mu'; \kappa). \quad (1.14)$$

Spectrum and Eigenfunctions of the Thermal Transport Operator

The fast neutron wave energy-dependent transport eigenvalue problem can best be introduced by discussing work which has been done on the analogous thermal problem, Eq. (1.14). This approach will be taken because transport treatment of the fast problem is necessary to obtain qualitatively correct spectral descriptions for passive media. Approximations such as diffusion theory can yield an estimate of the least attenuated mode of propagation in fast multiplying media, where such a fundamental mode exists, but can provide little other information relevant to the properties one should expect of the exact transport treatment.

The context of the work to be presented here is the "singular eigenfunction method," which received its major impetus from a paper by

Case [28], and thus is frequently known as "Case's method." As an introduction to the literature on the singular eigenfunction method in transport theory, including the wave problem, the review of McCormick and Kuščer [29] is highly recommended, as it is both recent and extensive.

Travelli [30] was the first investigator to arrive at an essentially correct description of the spectrum of the energy-dependent wave problem, based on a multigroup transport formulation. We turn now to the energy-dependent analysis of the thermal wave eigenvalue problem, corresponding to Eq. (1.14), performed independently by Kaper et al. [31] and Duderstadt [32,33]; the former study employs an isotropic one-term degenerate thermalization kernel, while Duderstadt discusses more general types of scattering interaction models as well. Their results are summarized in this section. Eq. (1.8) may be written in abbreviated form as

$$AF \equiv (A_1 + A_2)F = \kappa F \quad (1.15)$$

where the streaming operator A_1 is

$$A_1 \equiv \int_{-1}^1 d\mu' \int_0^\infty dE' \left(\frac{\Sigma_t(E)}{\mu} + \frac{i\omega}{\mu v(E)} \right) \delta(E' - E) \delta(\mu' - \mu) \cdot \quad (1.16)$$

and the interaction operator A_2 becomes

$$A_2 \equiv \int_{-1}^1 d\mu' \int_0^\infty dE' \frac{1}{\mu} \Sigma_S(E', \mu' \rightarrow E, \mu). \quad (1.17)$$

using the scattering interaction kernel of Eq. (1.14).

The basic method for obtaining the spectrum and eigenfunctions of this equation is a generalization of the work of Bednarz and Mika [34] on the static Boltzmann operator, which in turn extended the classic monoenergetic singular eigenfunction technique [25] to a continuous energy representation. We begin by defining the domain C in the spectral κ -plane, which is the continuous spectrum of the streaming operator A_1 :

$$C \equiv \left(\kappa \left| \frac{\Sigma_t(E)}{\mu} + \frac{i\omega}{\mu v(E)} - \kappa = 0, \mu \in [-1, 1], E \in [0, \infty) \right. \right) \quad (1.18)$$

or in the notation of Eq. (1.14), those values of κ for which $a - \mu\kappa$ vanishes. For any nonzero frequency ω , a is complex, so that C will occupy an area in the κ -plane. It is instructive to consider both the rectangular and polar forms of $\kappa \in C$; Eq. (1.18) implies that

$$\begin{aligned} \operatorname{Re}(\kappa) &\equiv \alpha = \frac{\Sigma_t(E)}{\mu} \\ \operatorname{Im}(\kappa) &\equiv \xi = \frac{\omega}{\mu v(E)} \\ r(\kappa) &= \frac{1}{\mu} \left(\Sigma_t^2 + \frac{\omega^2}{v^2} \right)^{1/2} \\ \theta(\kappa) &= \tan^{-1} \frac{\omega}{v \Sigma_t} \end{aligned} \quad (1.19)$$

where r and θ are the usual radial and azimuthal polar coordinates. In general C will consist of two symmetric portions in the first and third quadrants, due to $\mu \in (0,1]$ and $\mu \in (0,-1]$ respectively. This is represented schematically in Figure 1.1. Since frequency ω is a positive quantity, C does not extend into the second and fourth quadrants. Figure 1.2 shows the first quadrant of the κ -plane in more detail. The domain C is bounded by the line $\mu = \pm 1$, $\alpha = \Sigma_t$; from the rectangular form of Eq. (1.19) it is apparent that the real part of this boundary line assumes every value of Σ_t as E (and thus v) varies from 0 to ∞ . The polar form of Eq. (1.19) shows that as $|\mu|$ varies from 1 to 0, values of κ corresponding to a fixed E generate a line of constant θ which begins at the boundary of C and extends to infinity. As the parameter ω is increased or decreased the domain C expands or contracts in the imaginary κ direction.

We note that if $v\Sigma_t$ varies monotonically with E , each point of the domain C will correspond to a unique E, μ pair, E_κ and μ_κ ; for the thermal analysis presented here, this is assumed to be the case. Two important results then follow. First, Eq. (1.19) defines a one-to-one mapping of E, μ onto the spectral plane. Second, the spectrum of A_1 is not degenerate. The consequences of these results will be discussed later.

The discrete and residual spectra [35] of A_1 are empty [33]. The singular continuum eigenfunctions of A_1 , satisfying the equation

$$(A_1 - \kappa)F(E, \mu; \kappa) = 0 \quad (1.20)$$

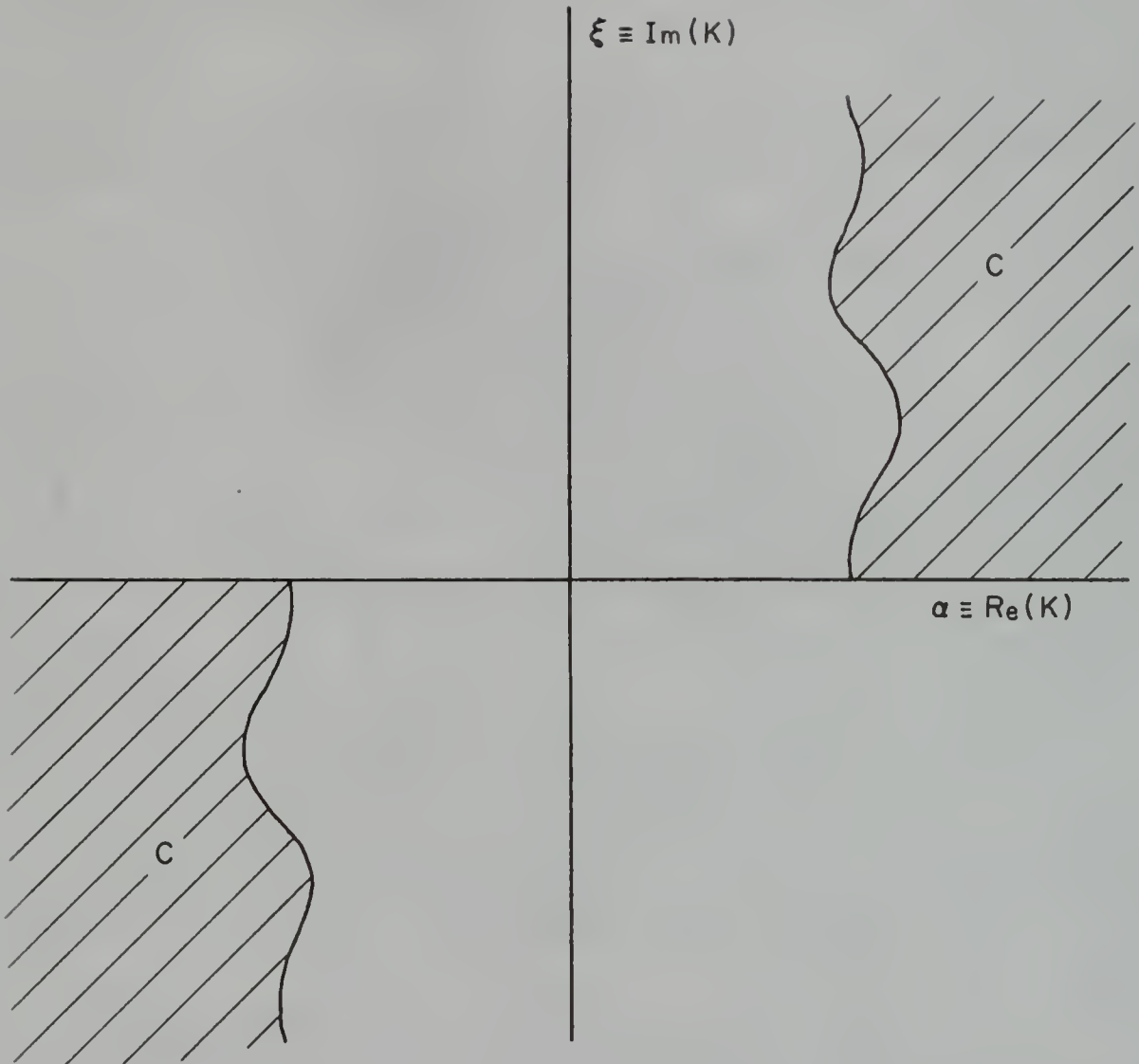


Figure 1.1 The continuum domain C in the spectral κ -plane.

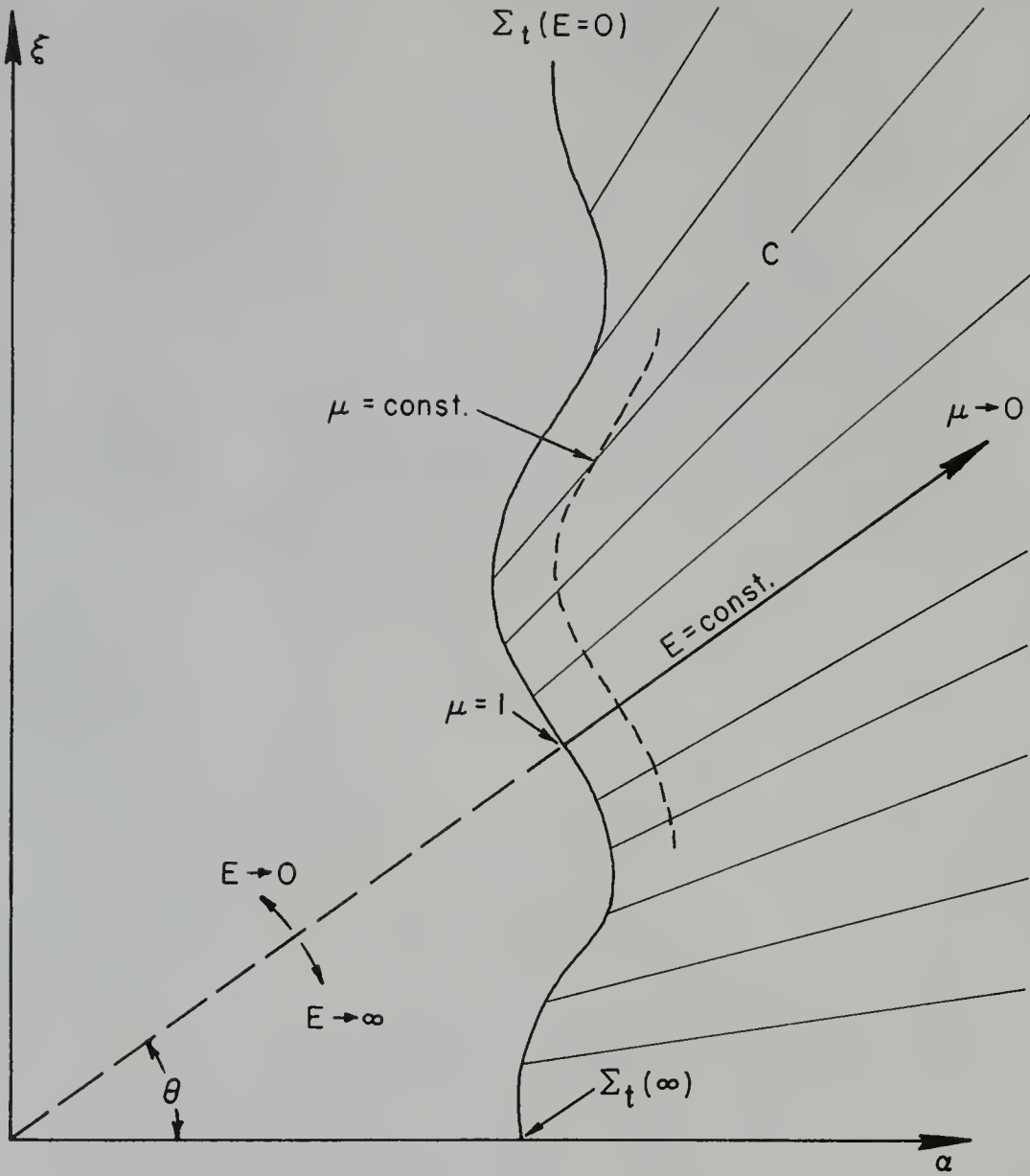


Figure 1.2 Structure of the continuum.

are

$$F(E, \mu; \kappa) \propto \delta(E - E_{\kappa}) \delta(\mu - \mu_{\kappa}) \equiv \delta(a - \mu \kappa) . \quad (1.21)$$

This gives a corresponding eigenmode, using Eq. (1.4) (for $A = A_1$),

$$\phi_{\kappa}(x, E, \mu, t) = e^{-\alpha x} e^{i(\omega t - \xi x)} \delta(E - E_{\kappa}) \delta(\mu - \mu_{\kappa}) \quad (1.22)$$

which clearly represents neutrons of energy E_{κ} streaming in the direction μ_{κ} . Since C is in one-to-one correspondence with all possible E, μ pairs, each point in the continuum corresponds to a unique neutron speed and direction of travel. Referring to Eq. (1.19) we see that modes with $\mu_{\kappa} = \pm 1$ have relaxation length $1/\Sigma_t(E_{\kappa})$ equal to the neutron relaxation length; that is, modes corresponding to κ on the boundary of C represent neutrons streaming along the x axis. Other modes are more attenuated, as the direction of neutron travel becomes more oblique to the direction of wave propagation.

The spectrum of the streaming operator and its eigenfunctions are qualitatively the same for both thermal and fast regimes, the only differences being the values of E which are applicable, and the detailed structure of Σ_t as a function of energy; Eqs. (1.19) - (1.22) apply in either case. It is the interaction operator A_2 , containing the description of the scattering and multiplication processes, which gives rise to the qualitative differences between fast and thermal WBE eigenfunctions.

It seems likely for "reasonable" mathematical models of thermal scattering that the spectrum of $A = A_1 + A_2$ always contains the spectrum

of A_1 . This has been substantiated for A_2 having the form of a separable kernel with isotropic scattering [31,33]. This model, which was proposed by Corngold et al. [36], has been used quite extensively in analytic transport studies, since it represents fairly well the qualitative features of thermal scattering interactions [37]. Duderstadt [33] has investigated more general operators A_2 , and while the spectral analysis for less restricted models is somewhat more tentative, it does appear to indicate that the spectrum of the streaming operator is in general contained in the spectrum of the wave Boltzmann operator A . We will see this in a more formal way from the technique used to construct the continuum eigenfunctions.

To illustrate this method we obtain the eigenfunctions for the thermal WBE with the separable isotropic thermalization kernel

$$A_2 = \frac{M(E)}{\mu} \int_{-1}^1 d\mu' \int_0^\infty dE' \Sigma_s(E') \cdot ,$$

$$\int_{-1}^1 d\mu \int_0^\infty dE M(E) = 1. \quad (1.23)$$

(To be consistent with our later treatment of the fast WBE we will not perform the usual symmetrization of this kernel, since for the fast case A_2 is not symmetrizable. The main result of interest which arises from symmetry of A_2 is that the eigenfunctions are mutually orthogonal, and one avoids the adjoint problem; this and other considerations will not be of direct concern here. Also note that $M(E)$ is not the Maxwellian

distribution. To satisfy detailed balance $M(E) = M'(E)\Sigma_S(E)$, where $M'(E)$ is proportional to the Maxwellian, subject to the above normalization constraint.)

Using this form for A_2 , the WBE corresponding to Eq. (1.14) becomes

$$(a-\mu\kappa)F(E,\mu;\kappa) = M(E) \int_{-1}^1 d\mu' \int_0^\infty dE' \Sigma_S(E')F(E',\mu';\kappa). \quad (1.24)$$

Notice that this expression is exactly equivalent to the fast multiplying WBE in the form of Eq. (1.13) when scattering is ignored in that equation. First we investigate the point spectrum. We see that κ will be an eigenvalue when the homogeneous equation (1.24) has a solution for that value of κ . Let us suppose that $\kappa \notin C$ so that $(a - \mu\kappa) \neq 0$; then dividing by this factor,

$$F(E,\mu;\kappa) = \frac{M(E)}{a-\mu\kappa} \int_{-1}^1 d\mu' \int_0^\infty dE' \Sigma_S(E')F(E',\mu';\kappa). \quad (1.25)$$

Defining the scalar product

$$(\phi(E,\mu), \psi(E,\mu)) \equiv \int_{-1}^1 d\mu \int_0^\infty dE \phi(E,\mu)\psi(E,\mu) \quad (1.26)$$

Eq. (1.25) may be written more compactly

$$F = \frac{M}{a-\mu\kappa} (\Sigma_s, F) \quad (1.27)$$

Taking the scalar product of this equation with Σ_s and eliminating the scalar factor (Σ_s, F) we find that the condition for Eq. (1.26) to have a solution is

$$1 = \left(\Sigma_s, \frac{M}{a-\mu\kappa} \right). \quad (1.28)$$

Defining the dispersion function

$$\Lambda(\kappa, \omega) \equiv 1 - \left(\Sigma_s, \frac{M}{a-\mu\kappa} \right), \quad (1.29)$$

Eq. (1.28) is simply the condition that this dispersion function vanish. Eq. (1.28), which is referred to as the dispersion law, determines in the present problem the regular eigenvalues κ of the WBE as a parametric function of frequency. Indeed, values of κ which satisfy the dispersion law for a given frequency ω have been shown [31,33] to comprise the point spectrum of A with A_2 defined by Eq. (1.23); for these eigenvalues κ_j the corresponding eigenfunctions are given by Eq. (1.27):

$$F(E, \mu; \kappa_j) = \lambda(\kappa_j) \frac{M(E)}{a-\mu\kappa} \quad (1.30)$$

where $\lambda(\kappa_j)$ is an arbitrary constant. (Note that for small ω and Σ_a this approaches a Maxwellian distribution in energy.)

When $\kappa \in C$, the term $(a - \mu\kappa)$ is zero for a particular $E = E_\kappa$ and $\mu = \mu_\kappa$. As we have mentioned, C is contained in the continuous spectrum. In the present case the continuous spectrum of A is identically the domain C , and the continuum eigenfunctions are [31,33,34]

$$F(E, \mu; \kappa) = \frac{M(E)}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^\infty dE' \Sigma_S(E') F(E', \mu'; \kappa) + \lambda(\kappa) \delta(a - \mu\kappa) \quad (1.31)$$

$$\kappa \in C$$

using the notation of Eq. (1.21); $\lambda(\kappa)$ is an arbitrary constant. We see that $(a - \mu\kappa)^{-1}$ has a pole at the "eigen-energy" E_κ and "eigen-angle" μ_κ ; integrals over E, μ involving this term will exist in the ordinary sense, provided that its coefficients in the integrand are well-behaved at the pole. Hence we may eliminate the scalar (Σ_S, F) in Eq. (1.31) in favor of the constant $\lambda(\kappa)$ by taking the scalar product of the equation with $\Sigma_S(E)$ and solving for (Σ_S, F) . We then find

$$F(E, \mu; \kappa) = \lambda(\kappa) \left[\frac{M(E)}{a - \mu\kappa} \frac{\Sigma_S(E_\kappa)}{\Lambda} + \delta(a - \mu\kappa) \right] \quad (1.32)$$

$$\kappa \in C$$

so that $\lambda(\kappa)$ is in fact a normalization constant; Λ is the dispersion function defined in Eq. (1.29)

Eq. (1.31) may be obtained directly from Eq. (1.24) by a heuristic argument [38]. Since for any variable x the function $x\delta(x)$ is identically zero, apparently $\lambda(a - \mu\kappa)\delta(a - \mu\kappa) \equiv 0$ may be added to the right-hand side of Eq. (1.24). Division by $(a - \mu\kappa)$ gives Eq. (1.31) when $\kappa \in C$. Evidently, then, the domain C always will be in the spectrum of A , since it is contributed by the streaming operator, regardless of the form of A_2 .

The continuum eigenfunction, Eq. (1.32), is composed of two singular terms, one being the pure streaming mode of Eq. (1.21), and the other having distributed E and μ dependence, with the same formal structure as the discrete eigenfunction, Eq. (1.30), except that it has a pole singularity since $\kappa \in C$. The scalar coefficient of the latter term, $\Sigma_s(E_\kappa)/\Lambda$, represents the relative excitation of the distributed portion of the mode by the streaming portion (this can be seen more clearly by comparing with the analogous fast continuum eigenfunction, which will be developed in Chapter II). Hence the continuum eigenfunction may be interpreted as being due to direct streaming neutrons having energy and direction E_κ and μ_κ , and an associated scattered distribution which is excited by the streaming neutrons; the scattered distribution is peaked at E_κ and μ_κ due to the pole of the transport coefficient $(a - \mu\kappa)^{-1}$, but contains all other E, μ values as well. Note, however, that the entire mode has the phase velocity $v_{ph} \equiv \frac{\omega}{\xi}$ (cf. Eq. (1.4)) of the uncollided wave. This interpretation of the thermal continuum eigenfunctions has not been given in previous treatments, as symmetrization of the kernel tends to obscure the physics involved.

Kaper et al. [31] have investigated the dispersion law $\Lambda = 0$ for the separable kernel model. Their findings may be summarized as follows. When $\omega = 0$, one has the classic exponential experiment [21]; there is exactly one pair of real eigenvalues $\kappa_j = \pm \kappa_p$, provided that the absorption of the medium is not too strong (of course the precise condition will depend on the energy dependence of the cross sections). Otherwise, the point spectrum is empty and will remain empty for all ω . As the parameter ω is increased from zero, the pair of eigenvalues will move symmetrically into the first and third quadrants of the complex κ -plane. Evidently for sufficiently large ω there will be a limiting frequency ω_c beyond which the discrete spectrum is empty; this value of frequency appears to occur when κ_p meets the boundary of the continuum C . This situation is represented schematically, for the first quadrant, in Figure 1.3. (We noted that in general the boundary of C is frequency-dependent; here for simplicity it is shown for Σ_t constant, in which case the boundary remains a line perpendicular to the real axis.)

While for a time it was conjectured [32,33] that zeroes of the dispersion function might exist within the continuum as "embedded eigenvalues" in a continuation of the dispersion law for $\omega > \omega_c$, it now appears [31,39] that this is not the case, although the dispersion function apparently does vanish at points within the continuum [39]; referring to Eq. (1.32), this corresponds to points at which the delta-function contribution vanishes. This subject will not be pursued here; the interested reader is referred to Kaper et al. [31], Klinc and Kušcer [39], and for an extensive discussion from a different point of view, to the work of Dorning and Thurber [40] and Dorning [41].

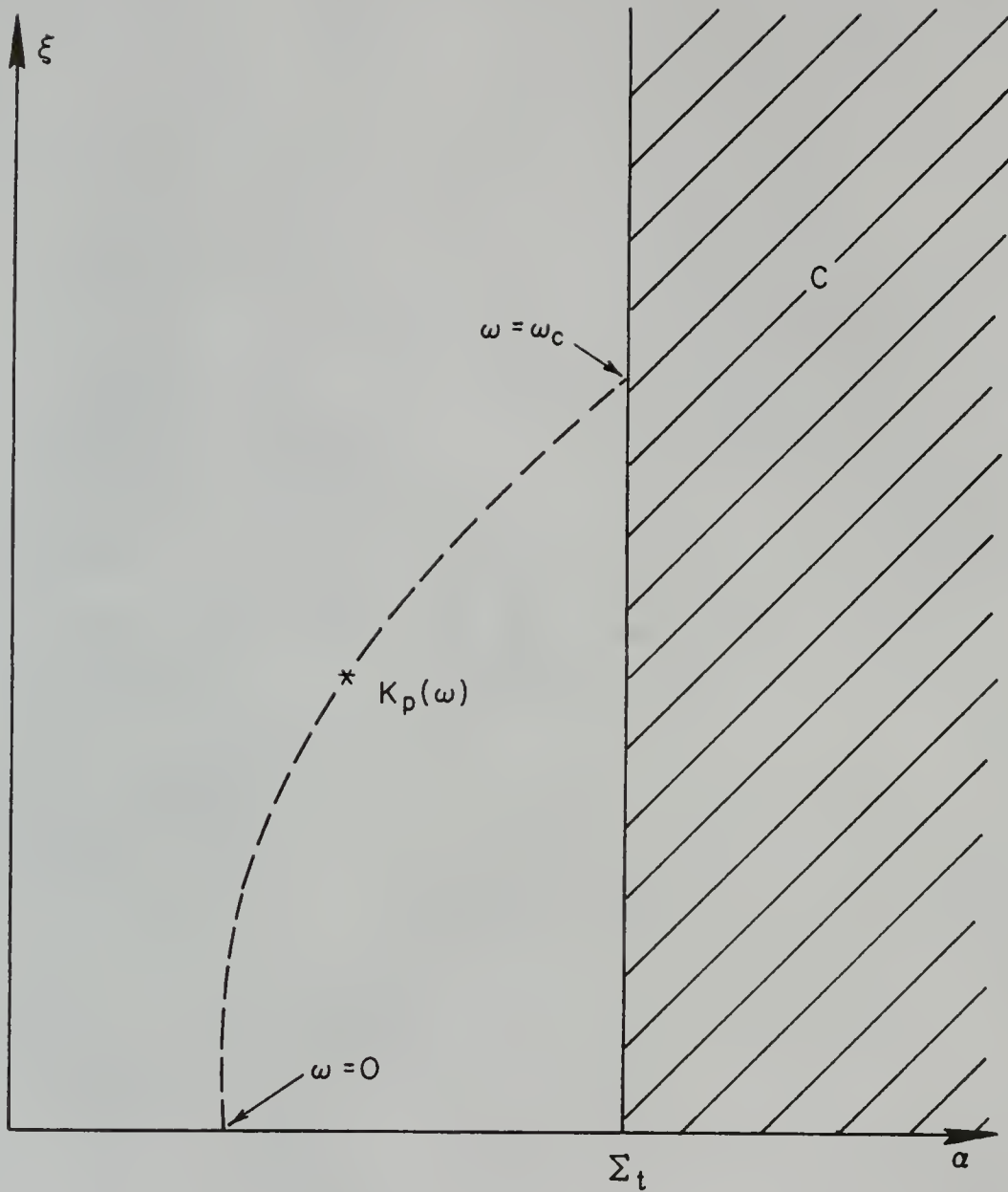


Figure 1.3 Schematic dispersion law for a discrete eigenvalue.

From the results of calculations based on the separable kernel or comparable models [31,32] it is possible to draw some conclusions about the physical interpretation of the frequency-dependent behavior of the dispersion law. Near zero frequency the fundamental neutron wave mode (if there is one) corresponding to $\pm \kappa_p$ is less attenuated than the streaming-associated continuum modes. As ω increases, the wavelength of the fundamental mode decreases and it becomes more attenuated. This occurs because it becomes increasingly difficult for scattered neutrons to remain in phase with the wave; from Eq. (1.24) we see that as κ_p approaches C the energy and angular distributions of the wave become increasingly peaked for $\mu = \pm 1$. Ultimately the fundamental mode becomes nearly as attenuated as forward-streaming neutrons, and evidently the distributed E, μ term of the continuum eigenfunctions then assumes the role formerly held by the fundamental mode as the frequency increases beyond ω_c .

One additional remark should be made. For $\omega = 0$ the spectrum of the static Boltzmann equation lies entirely on the real axis, and in general it appears that it is the limit of the spectrum of the WBE as ω approaches zero. But obviously for κ real the identification of E, μ pairs with points of C no longer can be made. Indeed it may be improper to regard the static Boltzmann equation as the zero-frequency limit of the WBE. No such problem arises in connection with the discrete spectrum, in the sense that in the limit $\omega = 0$, Eq. (1.28) gives the correct eigenvalues for the static case. This evidently is true of the dispersion law in general, and in that sense we speak loosely of the exponential experiment being the zero-frequency limit of the wave experiment.

In this work we will be concerned only with $\omega \neq 0$ except in the calculations of Chapter IV, which involve only the discrete eigenvalues and eigenfunctions.

Completeness of the Thermal Eigenfunctions

In order to make use of a set of eigenfunctions such as those obtained in the previous section, it is necessary to show that arbitrary functions (suitably restricted) can be expanded using these functions as a basis, and it is further necessary to evaluate the expansion coefficients. First, then, one must prove that the set of eigenfunctions is complete, or at least establish completeness within the context of the problem one is to consider. Then either the eigenfunctions must be shown to be orthogonal and normalized to unity scalar product, so that orthogonality properties may be used to obtain expansion coefficients in the usual way, or some other procedure must be followed. Normalization of continuum eigenfunctions is somewhat less than straightforward because, as may be seen from the form of these eigenfunctions in Eq. (1.32), it involves products of delta functions of complex variables. The alternative procedure is to find the continuum expansion coefficients $G(\kappa)$ of an arbitrary function $\Psi(E, \mu)$ directly from the expression for the expansion, which is a singular integral equation:

$$\Psi(E, \mu) = \iint_{\kappa} G(\kappa) F(E, \mu; \kappa) d\kappa \quad (1.33)$$

where Ψ^{\wedge} is the portion of Ψ contributed by the continuum eigenfunctions (the discrete mode contribution is found by the usual application of orthogonality). $F(E, \mu; \kappa)$, which is now the kernel of the integral operator, is known from Eq. (1.32) or a similar evaluation of the continuum eigenfunction based on another model.

In implementing either method the theory of generalized analytic functions [42] has been the principle tool applied to date. Eq. (1.33) also has been used to prove completeness of the WBE eigenfunctions, since if it can be shown that an arbitrary $\Psi(E, \mu)$ has a representation in this form, the set of eigenfunctions $F(E, \mu; \kappa)$ must be complete. This approach has been taken by Kaper et al. [31] and Duderstadt [32] to show completeness for the eigenfunctions of the separable thermalization model of the previous section; their treatments were based on extension of the generalized analytic function technique as applied by Cercignani [43] to problems in the kinetic theory of gases. The details of this analysis are lengthy and will not be repeated here.

We will make reference to two types of completeness and orthogonality. We note that values of κ in the first quadrant correspond to plane waves propagating in the positive x direction, and similarly the third quadrant represents waves propagating in the negative x direction. In general, e.g., within a slab of finite thickness, a wave will be made up of components traveling in both directions; to represent an arbitrary wave (or pulse frequency component) $\Psi(E, \mu, x, \omega)$ in WBE eigenfunctions, one must use all the eigenfunctions, corresponding to the whole spectrum of the wave Boltzmann operator. Completeness of the first type, in the sense that a unique representation of this sort can

be made, is termed full-range completeness. The corresponding full-range orthogonality is simply orthogonality under the scalar product of Eq. (1.26).

In applying eigenfunction techniques to boundary value problems, one frequently wishes to represent an incoming source flux $S(E, \mu, x_0, \omega)$ or to specify flux continuity for waves moving from one region into another across an interface at a boundary point x_0 . In this case the boundary condition will be specified for either $\mu \in [-1, 0)$ or $\mu \in (0, 1]$ and will involve eigenfunctions for only one direction of wave propagation. Completeness in this sense, termed half-range completeness, requires that a function defined over $\mu \in (0, 1]$ or $\mu \in [-1, 0)$ can be represented uniquely by WBE eigenfunctions corresponding to the eigenvalues in only the first or third quadrant of the spectral plane, respectively. Half-range orthogonality is orthogonality under integration the half range of μ .

Both full-range and half-range completeness requirements will be seen to arise in Chapter III in connection with a formalized treatment of the slab geometry boundary value problem. We should note that at present half-range completeness can be proved only for quite restricted kernel models, although full-range completeness can be shown for more general kernels [29,33]. Our main interest in the completeness properties of the eigenfunctions of Eqs. (1.24) and (1.26) is that they are indeed complete. We will use the same formal procedure to find the eigenfunctions of the fast WBE, and will obtain qualitatively similar results. Thus we may have considerable confidence, in lieu of proof, that the fast eigenfunctions are complete as well.

There are two difficulties which will prevent us from extending the generalized analytic function technique directly to the fast regime. First, one must deal with the slowing-down operator. Second, the one-to-one equivalence between values of E, μ and points of C does not hold for realistic fast cross sections (e.g., at resonances), and we will be reluctant to consider more restrictive cross-section models (i.e., monotonic $v\Sigma_t$); this equivalence plays a central part in the generalized analytic function method as it has been developed to date. Whether these two problems are insurmountable is a matter for further investigation; however, it seems unlikely, in view of the results established in the thermal case, that the fast eigenfunctions would not be complete for "reasonable" cross-section models. (An example of an "unreasonable" model is a strictly $1/v$ -dependent cross section

$$\Sigma_t(E) = \frac{\Sigma_t^0}{v}$$

or one which has this behavior over some energy range. When this occurs the portion of C corresponding to this energy range collapses onto a line. This case is discussed for thermal waves in polycrystalline material by Duderstadt [33] and by Yamagishi [44]; it is necessary to deal separately with the eigenfunctions on the line continuum which results from this cross section.)

For an introduction to other literature on completeness of singular eigenfunctions see the review of McCormick and Kuščer. It is interesting in this connection to read the comments of Burniston et al. [45], and

the recent remarks of Zweifel [46] regarding the degree to which the rigorous mathematical basis for the singular eigenfunction transport analysis has been established.

Other Related Problems and Literature

In the foregoing discussion we have seen that for the thermalization model employed there the spatially dominant wave mode is due to the regular eigenvalue κ_p , which is determined by the zeroes of the dispersion function $\Lambda(\kappa, \omega)$. Further, we see from Eq. (1.32) that the zeroes or near-zeroes of Λ also will play a large part in determining the character of continuum modes, since in regions where Λ is small the scattering portion of the mode will dominate the streaming term. A corresponding dispersion function appears to arise in general in the treatment of regenerative media (i.e. those in which neutron interactions can result in either a gain or loss in energy, and hence the interaction kernel has a Fredholm form). Dorning and Thurber [40], for example, find that in an alternative formulation of the wave problem and in an initial value problem the nature of solutions is similarly influenced by the behavior of a dispersion function. In addition, dispersion laws are known to arise in nontransport approximations to dynamic eigenvalue problems. For example, when the multi-group diffusion approximation is used to obtain a matrix expression analogous to Eq. (1.8), its determinant is the dispersion function, and the dispersion law is simply the requirement that the determinant vanish; the solutions associated with values of κ which satisfy the dispersion law are then the desired eigenmodes. Indeed the multi-group diffusion

approach has been used rather extensively to compute dispersion laws for moderators, and when sufficiently accurate scattering matrices are employed, agreement of diffusion theory methods with experiment at low frequencies can be quite good [47].

General discussions of wave and pulse propagation in the context of its relationship to other dynamic problems, properties of the various dispersion laws, and analytic methods which have been applied to these problems will be found in Bell and Glasstone [21] and Hetrick [48]. An excellent review of the literature in this area as of 1967 has been given by Kušč^ˇer [49], although it is of course somewhat dated. As an alternative exact approach to transport problems, the Wiener-Hopf technique is finding increasing favor and must be viewed as a potential method for analysis of the wave problem; Williams [50] recently has published an expository review of the method. Also, the singular eigenfunction method review of McCormick and Kušč^ˇer [29] should be mentioned again in connection with the subject of transport treatments of various static and dynamic problems.

Finally, with respect to the subject of Chapter III, note should be taken of existing work treating neutron waves in geometry which is finite or has discontinuities along the direction of wave propagation. Interface effects first were investigated experimentally by Denning, Booth and Perez [51]. This same problem was the subject of both numerical and analytic investigation by Baldonado and Erdmann [52,53]; their work is of particular interest because one-speed and energy-dependent diffusion and transport results are given. Mockel [54] has presented both transfer matrix and invariant imbedding transport formulations for

wave transmission and reflection from a slab imbedded in an infinite medium of different composition. Also to be noted is the treatment of Larson and McCormick [55] of transport in a slab, in the static case, using a degenerate scattering kernel. Recently much attention has been given by Japanese and Indian groups to the problem of thermal neutron wave propagation in assemblies of polycrystalline moderating materials (e.g. graphite and beryllium) having finite transverse and longitudinal dimensions; see for example Nishina and Akcasu [56], Kumar et al. [57], and Yamagishi [44]. The latter is of particular interest because it demonstrates, in a transport treatment, the presence of intermodal interference.

CHAPTER II

SPECTRUM AND EIGENFUNCTIONS OF THE FAST WAVE TRANSPORT OPERATOR

Introduction

In this chapter the singular eigenfunction formalism, presented in Chapter I, will be extended to the fast WBE expressions, Eqs. (1.12) and (1.13). Both the forward and adjoint eigenfunctions will be obtained for general forms of the nonmultiplying, or "slowing-down," and multiplying cases. The structure of these solutions will be discussed, and some of the implications of using realistic cross-section and scattering kernel models will be explored.

Adjoint eigenfunctions will be investigated for two reasons. First, they will be necessary for the treatment of the transport formulation of the transfer matrix in Chapter III. Second, as has been mentioned, analytic evaluation of expansion coefficients cannot be performed using generalized analytic function techniques which have been applied to thermal problems. For the same reason, we will not obtain normalization constants analytically. However, biorthogonality of eigenfunction sets will be shown in the classic way.

Adjoint Eigenfunction Equations

The appropriate scalar product under which to define adjoint operators is given by Eq. (1.26). We consider the general wave eigenvalue

equation in the form of Eq. (1.8), which we may write as

$$\frac{a}{\mu} F(E, \mu; \kappa) - \frac{1}{\mu} \int_{-1}^1 d\mu' \int_0^{\infty} dE' K(E', \mu' \rightarrow E, \mu) F(E', \mu'; \kappa) = \kappa F(E, \mu; \kappa). \quad (2.1)$$

The adjoint eigenfunctions will be denoted by $F^{-1}(\kappa; E, \mu)$; the adjoint eigenvalue equation corresponding to the forward equation, Eq. (2.1), is

$$\frac{a}{\mu} F^{-1}(\kappa; E, \mu) - \int_{-1}^1 d\mu' \int_0^{\infty} dE' \frac{1}{\mu'} K(E, \mu \rightarrow E', \mu') F^{-1}(\kappa; E', \mu') = \kappa F^{-1}(\kappa; E, \mu) \quad (2.2)$$

where we notice the factor $\frac{1}{\mu}$ is now within the integral. However, if we define

$$F^{\dagger}(\kappa; E, \mu) \equiv \frac{1}{\mu} F^{-1}(\kappa; E, \mu) \quad (2.3)$$

Eq. (2.2), becomes, upon substitution and rearranging,

$$(a - \mu\kappa) F^{\dagger}(\kappa; E, \mu) - \int_{-1}^1 d\mu' \int_0^{\infty} dE' K(E, \mu \rightarrow E', \mu') F^{\dagger}(\kappa; E', \mu') = 0 \quad (2.4)$$

which is the form which would have been obtained as the adjoint of the homogeneous wave Boltzmann equation, Eq. (1.7). It will be more convenient to deal with Eq. (2.4) since it differs from the forward WBE, Eq. (1.7), only in the kernel of the interaction operator and hence we

will be able to apply the same techniques to the solution of both forward and adjoint equations.

It should be pointed out that κ is used for the eigenvalue in Eq. (2.2), with the implication that the spectra for forward and adjoint equations are identical. That this is true for "well-behaved" operators in the models we are considering will be apparent from the singular eigenfunction formalism, although of course each case must be explained individually. Nicolaenko [14] has exhibited an inelastic scattering operator for which the adjoint spectrum contains additional contributions due to a singularity of the kernel at zero energy; he uses the singular kernel in defining an energy transform for reduction of the static transport slowing-down equation (for the model he considers) to monoenergetic form. However it is shown in Appendix B that singularity of inelastic scattering kernels is not an inherent attribute of fast neutron transport problems. Thus for the forward and adjoint problems the spectra and eigenfunctions can be regarded tentatively as being in correspondence, subject to verification for specific interaction models.

Biorthogonality of Eigenfunctions

Biorthogonality of WBE eigenfunctions corresponding to different eigenvalues can be shown by the usual argument. Writing Eq. (2.4) for κ' and Eq. (1.7) for κ , we take scalar products of the two equations with $F(\kappa)$ and $F^\dagger(\kappa')$ respectively, and subtract to find

$$(\kappa - \kappa') \left(\mu F^\dagger(\kappa'), F(\kappa) \right) = 0, \quad (2.5)$$

noting that we are using a real-type scalar product, Eq. (1.26). We conclude that biorthogonality holds for F^\dagger and F under a μ -weighted scalar product, while in view of Eq. (2.3) this is equivalent to biorthogonality of F^{-1} and F with unit weighting.

Nonmultiplying Media: Spectrum of the Slowing-Down Transport Operator

In fast nonmultiplying media the WBE is given by Eq. (1.12). The corresponding adjoint WBE, Eq. (2.4), is found to be

$$(a - \mu\kappa)F^\dagger(\kappa; E, \mu) = \int_{-1}^1 d\mu' \int_0^E dE' \Sigma_S(E, \mu \rightarrow E', \mu')F^\dagger(\kappa; E', \mu') \quad (2.6)$$

where the different energy limits for the adjoint Volterra scattering operator are to be noted.

We have seen in Chapter I that for the absorption-only case

$$(a - \mu\kappa)F(E, \mu; \kappa) = 0 \quad (2.7)$$

the spectrum is the domain C in which $(a - \mu\kappa)$ vanishes. The singular eigenfunctions were

$$F(E, \mu; \kappa) = F^\dagger(\kappa; E, \mu) = \lambda(\kappa)\delta(a - \mu\kappa) \quad (2.8)$$

where the second identity occurs since Eq. (2.7), the streaming equation, is self-adjoint. Thus in the limit of no scattering, the eigenfunctions of the fast WBE tend to the delta-function form, Eq. (2.8).

We observe from Eqs. (1.7) and (2.6) that the domain C , due to the streaming operator, also is contained in the continuous spectrum for the slowing-down WBE; we now show that in fact it is identically the spectrum since the scattering operator will cause no additional contribution to the spectrum. To demonstrate this we show that all $\kappa \notin C$ are in the resolvent set, which is the complement of the spectrum, and is defined as those values of κ for which $(A - \kappa)$ has a bounded inverse. Therefore we consider the existence of solutions to the equation

$$(A - \kappa)\phi = s(E, \mu). \quad (2.9)$$

We examine first the case of isotropic scattering, for which the scattering operator becomes

$$\int_{-1}^1 d\mu' \int_E^\infty dE' \Sigma_S(E', \mu' \rightarrow E, \mu) \cdot = \int_{-1}^1 d\mu' \int_E^\infty dE' \frac{1}{2} \Sigma_S(E' \rightarrow E) \cdot \quad (2.10)$$

Using this operator we may write for Eq. (2.9) the equivalent equation

$$(a - \mu\kappa)\phi(E, \mu) - \int_{-1}^1 d\mu' \int_E^\infty dE' \frac{1}{2} \Sigma_S(E' \rightarrow E)\phi(E', \mu') = S(E, \mu). \quad (2.11)$$

For values of $\kappa \notin C$ we may divide by $(a - \mu\kappa)$ and integrate over μ :

$$\begin{aligned}
\int_{-1}^1 \phi(E, \mu) d\mu &\equiv \phi(E) \\
&= \int_{-1}^1 \frac{d\mu}{a - \mu\kappa} \int_E^{\infty} dE' \frac{1}{2} \Sigma_S(E' \rightarrow E) \phi(E') + \\
&\quad + \int_{-1}^1 d\mu \frac{S(E, \mu)}{a - \mu\kappa} .
\end{aligned} \tag{2.12}$$

Since $\kappa \notin \mathbb{C}$, both integrals over μ exist and Eq. (2.10) is of the form

$$\phi(E) = f(E) \int_E^{\infty} dE' \frac{1}{2} \Sigma_S(E' \rightarrow E) \phi(E') + g(E) \tag{2.13}$$

or

$$\left(1 - f(E) \int_E^{\infty} dE' \frac{1}{2} \Sigma_S(E' - E) \cdot \right) \phi(E) = g(E) . \tag{2.14}$$

Provided that the scattering kernel is bounded, the Neumann series inverse

$$\phi(E) = \sum_{n=0}^{\infty} \left(f(E) \int_E^{\infty} dE' \frac{1}{2} \Sigma_S(E' \rightarrow E) \cdot \right)^n g(E) \tag{2.15}$$

always exists [58]. Thus $(A - \kappa)$ has a bounded inverse, and we have

the result that the complement of C is not in the spectrum of A . An identical argument applies to the adjoint operator.

We can extend this result to anisotropic scattering by making a P_N expansion of the scattering kernel and ϕ ; the procedure of Eq. (2.12) then results in a set of coupled Volterra equations which must be inverted. Thus for rather general scattering kernels, i.e., those which can be developed in a finite bounded P_N expansion, we have the result that the spectrum of the wave Boltzmann operator consists only of the continuum C .

Forward and Adjoint Slowing-Down Eigenfunctions

Since the point spectrum for the slowing-down problem is empty, there will be no regular eigenfunctions and corresponding space- and E, μ -separable eigenmodes. To obtain the singular eigenfunctions corresponding to the continuous spectrum $\kappa \in C$, we may apply the technique of Chapter I. Adding $\lambda(\kappa)(a - \mu\kappa)\delta(a - \mu\kappa)$ to the right-hand side of Eq. (1.12) and dividing by $(a - \mu\kappa)$ we find

$$F(E, \mu; \kappa) = \frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_E^\infty dE' \Sigma_S(E', \mu' \rightarrow E, \mu) F(E, \mu; \kappa) +$$

$$+ \lambda(\kappa)\delta(a - \mu\kappa), \quad \kappa \in C$$

(2.16)

or equivalently,

$$\left(1 - \frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_E^\infty dE' \Sigma_S(E', \mu' \rightarrow E, \mu) \cdot \right) F(E, \mu; \kappa) = \lambda(\kappa) \delta(a - \mu\kappa). \quad (2.17)$$

At this point it is necessary to proceed more formally. It has been observed in Chapter I that the integral of the factor $(a - \mu\kappa)^{-1}$ over E, μ exists, since it is a pole. We would like to extend the Neumann series inverse, which we used in Eq. (2.15), to Eq. (2.17). Accordingly we write

$$\begin{aligned} F(E, \mu; \kappa) &= \lambda(\kappa) \sum_{n=0}^{\infty} \left(\frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_E^\infty dE' \Sigma_S(E', \mu' \rightarrow E, \mu) \cdot \right)^n \delta(a - \mu\kappa) \\ &\equiv \lambda(\kappa) \mathcal{S} \cdot \delta(a - \mu\kappa) \\ &\equiv F_{SD}(E, \mu; \kappa) \end{aligned} \quad \kappa \in \mathbb{C} \quad (2.18)$$

as the forward slowing-down eigenfunction. The formal "Case's Method" derivation of Eq. (2.16) must be verified for specific scattering kernel models by means of more careful arguments such as those used in substantiating Eq. (1.32) [31,33,34]; it appears that this will succeed for "well-behaved" scattering kernel models. For κ in the continuous spectrum of A the inverse of the operator $(A - \kappa)$ exists but is singular [35], so it is with some justification that we write the second form of

Eq. (2.18), defining the formal inverse scattering operator \mathcal{S} . Further, the Neumann series expansion has an interesting physical interpretation in terms of familiar iterated collision integrals.

To see this we first recall that the zero scattering cross-section eigenfunction of Eqs. (1.21) and (2.8) represent neutrons streaming with eigen-energy E_{κ} and direction μ_{κ} ; this delta-function distribution is also the $n = 0$ term of $F(E, \mu; \kappa)$. The second term is

$$\begin{aligned}
 F^{(1)}(E, \mu; \kappa) &\propto \frac{1}{a - \mu\kappa} \Sigma_s(E_{\kappa}, \mu_{\kappa} \rightarrow E, \mu) & E < E_{\kappa} \\
 &= 0 & E > E_{\kappa}
 \end{aligned} \tag{2.19}$$

which may be interpreted as the distribution resulting from one down-scattering interaction, multiplied by the transport factor $(a - \mu\kappa)^{-1}$ which is peaked at E_{κ} and μ_{κ} . Similarly, higher terms in the expansion may be interpreted as the result of n down-scattering interactions, so that the entire eigenfunction may be regarded as the result of excitation by neutron waves streaming with E_{κ} and μ_{κ} , along with an associated down-scattered contribution excited by the streaming portion. The eigenfunction is nonzero only for E_{κ} and below, since only down-scattering can occur. (This deduction from Eq. (2.18) is valid whether the Neumann series converges for $E < E_{\kappa}$ or not.) We see that the eigenfunction singularity consists of a delta-function contribution and a pole contribution at E_{κ} ; a similar structure occurs in the thermal continuum eigenfunction, Eq. (1.32). Also we note that in the iterated

integrals each singularity is smoothed by integration, and that the unintegrated pole can be factored out from each term of the series, so that we suspect that the Neumann series inverse will indeed converge for rather general classes of scattering kernels.

The adjoint eigenfunctions may be obtained by an identical procedure; Eq. (2.6) leads to

$$\begin{aligned}
 F^\dagger(\kappa; E, \mu) &= \lambda^\dagger(\kappa) \sum_{n=0}^{\infty} \left[\frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^E dE' \Sigma_S(E, \mu \rightarrow E', \mu') \right]^n \delta(a - \mu\kappa) \\
 &= \lambda^\dagger(\kappa) \delta^\dagger \cdot \delta(a - \mu\kappa) \quad \kappa \in \mathbb{C}
 \end{aligned} \tag{2.20}$$

or

$$F^\dagger(\kappa; E, \mu) \equiv F_{SD}^\dagger(\kappa; E, \mu) \tag{2.21}$$

where $\lambda^\dagger(\kappa)$ is an arbitrary complex constant. The form of the adjoint Volterra operator requires that F^\dagger is identically zero for $E < E_\kappa$; again the delta-function and scattering-associated term with pole singularity at $E = E_\kappa$ occur. The properties of the forward and adjoint eigenfunctions may be summarized by the rearranged expressions

$$\begin{aligned}
F(E, \mu; \kappa) &= \lambda(\kappa) \left[\delta(a - \mu\kappa) + \right. \\
&+ \frac{1}{a - \mu\kappa} \sum_{n=0}^{\infty} \left(\int_{-1}^1 d\mu' \int_E^{E_K} dE' \frac{\Sigma_S(E', \mu' \rightarrow E, \mu)}{a(E') - \mu\kappa} \cdot \right)^n \times \\
&\quad \times \Sigma_S(E_K, \mu_K \rightarrow E', \mu') \Big] , \\
&\quad E \leq E_K \\
= 0 &\quad E > E_K \tag{2.22}
\end{aligned}$$

$$\begin{aligned}
F^\dagger(\kappa; E, \mu) &= \lambda^\dagger(\kappa) \left[\delta(a - \mu\kappa) + \right. \\
&+ \frac{1}{a - \mu\kappa} \sum_{n=0}^{\infty} \left(\int_{-1}^1 d\mu' \int_{E_K}^E dE' \frac{\Sigma_S(E, \mu \rightarrow E', \mu')}{a(E') - \mu\kappa} \cdot \right)^n \times \\
&\quad \times \Sigma_S(E', \mu' \rightarrow E_K, \mu_K) \Big] , \\
&\quad E \geq E_K \\
= 0 &\quad E < E_K . \tag{2.23}
\end{aligned}$$

Discussion of the Slowing-Down Eigenfunctions

An interpretation of the forward eigenfunctions in terms of iterated collision integrals excited by monoenergetic unidirectional (i.e. $\mu = \mu_{\kappa}$) streaming neutrons already has been given. We proceed by considering their biorthogonality properties. In general, due to the condition expressed by Eq. (2.5), forward and adjoint eigenfunction pairs corresponding to different eigenvalues are orthogonal under a μ -weighed scalar product. For the same eigenvalue κ , Eqs. (2.22) and (2.23) clearly show that the scalar product will not vanish, due to the coincident delta-functions. (This product of delta-functions of two variables requires careful interpretation in terms of the theory of generalized analytic functions or some other approach; for an introduction to the literature on this aspect of the singular eigenfunction technique see McCormick and Kuščer.[29].) The biorthogonality properties of the slowing-down eigenfunctions are illustrated schematically in Figure 2.1 in terms of the energy variable. The eigenfunctions must be orthogonal for overlapping energy-distributions as well as in the trivial case when the distributions are nonoverlapping in energy.

It is interesting to consider the expansion of a monoenergetic source in slowing-down eigenfunctions. This is schematically represented in Figure 2.2. We see from the first two sketches that such a source will excite not only continuum modes having the eigen-energy E_0 , but also will excite to some extent all modes with lower eigen-energies. As is apparent in the third sketch, continuum modes with higher eigen-energies will not be excited.

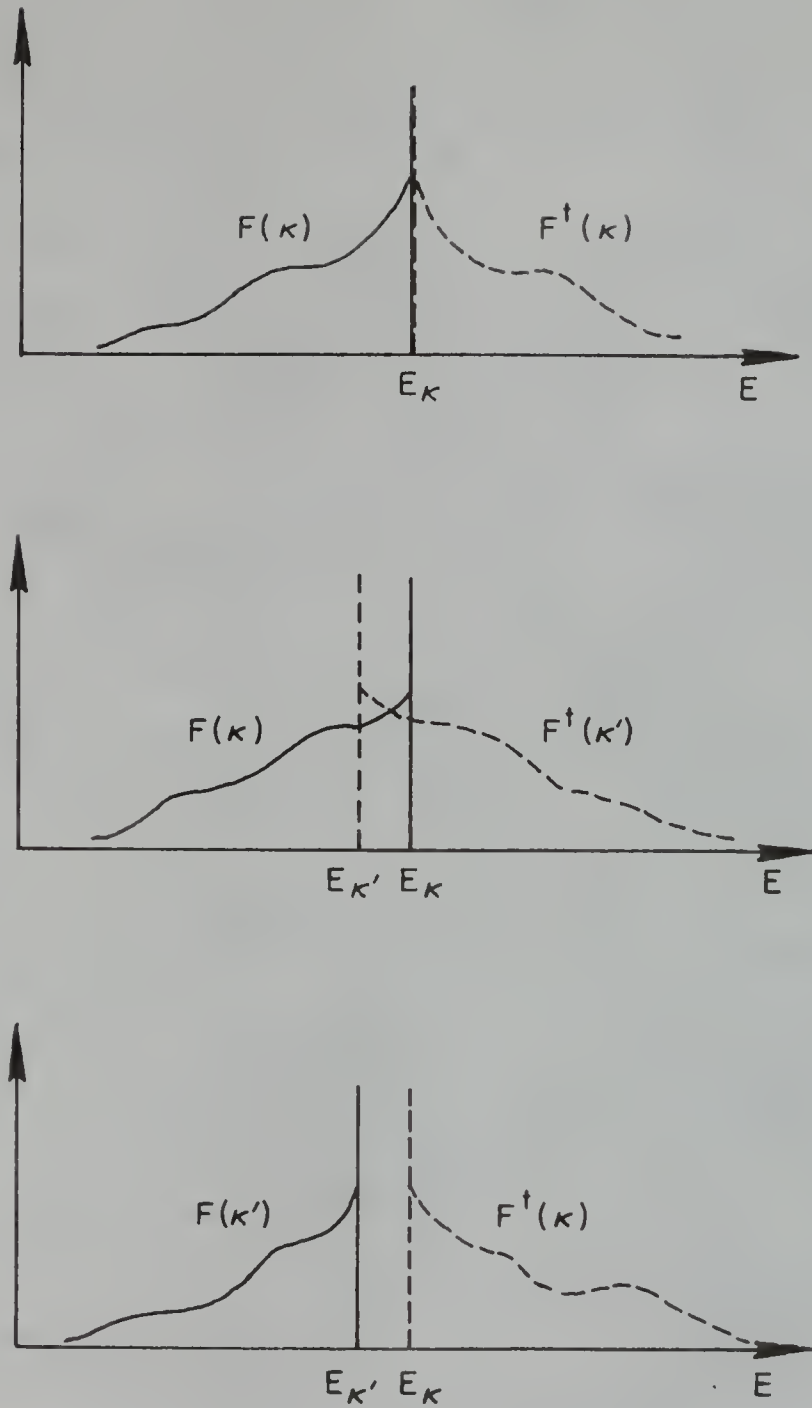


Figure 2.1 Orthogonality of forward and adjoint slowing-down eigenfunctions.

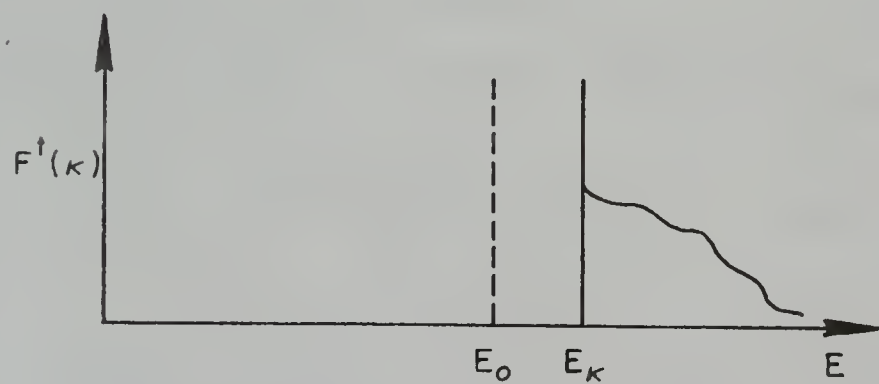
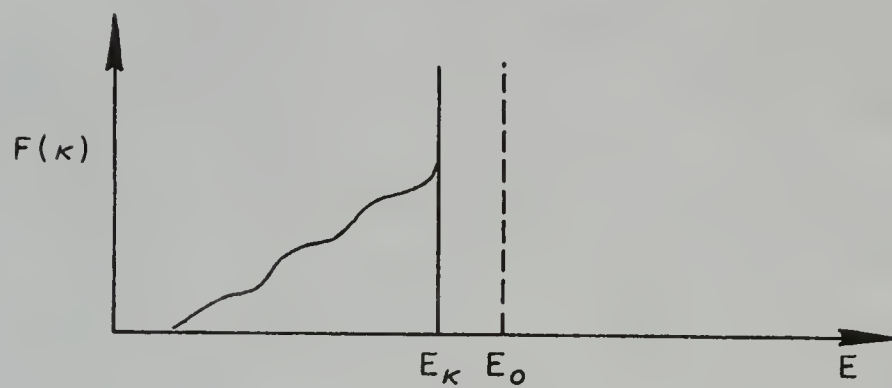
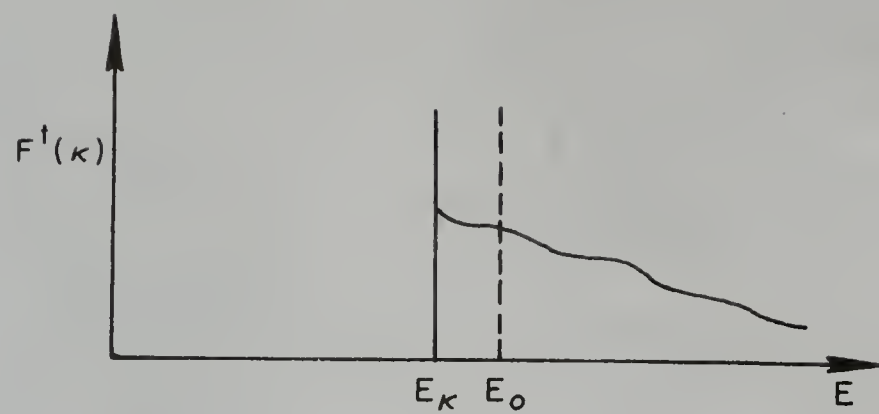


Figure 2.2 Excitation of slowing-down eigenfunctions by a monoenergetic source.

An analysis of the static slowing-down transport equation has been performed by MacInerney [59] for constant cross sections and elastic scattering, in the lethargy variable. By performing a lethargy Laplace transform he reduces the lethargy-dependent problem to one-speed transport form. For the transformed problem (for slowing down in hydrogen) both discrete and continuous spectra arise, as is usual in the one-speed problem (see standard works such as Case and Zweifel [25]). However due to inversion of the lethargy transform, the discrete modal contribution fails to give a space-separable solution for the isotropic space and lethargy Green's function (i.e. a source $\delta(u)\delta(x)$). This is in accord with our result that a monoenergetic source excites a continuous distribution of eigenfunctions. MacInerney tentatively attributes his continuum eigenfunctions to streaming first-flight source neutrons; confirmation of this, and further correlations between his work and the present "exact" method must await more detailed investigation.

The existence of a discrete mode in the lethargy-transformed problem raises an interesting point with respect to implementation of the continuum singular eigenfunctions. A dispersion function, associated with both discrete and continuum modes, was seen to arise naturally in the treatment of the thermal problem. We may associate the dispersion function with inversion of the Fredholm thermalization operator, since in the slowing-down case only the Volterra operator is present, and no such dispersion function appears. Physically we distinguish between energy-regeneration which can occur through up-scatter in the former instance and energy degradation in the latter. In the presence

of energy-regenerative mechanisms we find the potential for establishment of E, μ -space-separable modes (for moderate frequencies and absorptions) with attenuation length longer than the neutron mean free path. For the slowing-down problem, with such mechanisms absent we have

$$\xi = \text{Re } \kappa = \frac{\Sigma_t(E_\kappa)}{\mu_\kappa} \quad (2.24)$$

so that all modes are attenuated precisely as are the streaming-waves with which we associate them.

However it is well known that the neutrons themselves (e.g. for neutron pulses) are not attenuated in this manner, even though no separable mode of propagation exists. Evidently, therefore, we are not to regard a continuum mode as observable or capable of being excited individually, since the neutrons which would constitute such a wave certainly would not be attenuated according to the streaming mean free path. This is further evidenced by the fact that a monoenergetic unidirectional source excites modes having lower eigen-energies as well. Apparently the identification of an individual mode with streaming and associated scattered neutrons must be applied with some caution, although it is clear that actual streaming source neutrons are represented by the delta-function term of the appropriate eigenfunction. We must conclude that the spatially persistent nonseparable neutron population (as opposed to uncollided neutrons) excited by a delta-function source is represented by constructively interfering continuum eigenfunctions, where this constructive interference is due both to the distributed

part of the eigenfunction excited by the streaming, and to eigenfunctions of lower eigen-energies. Evidently the discrete mode in MacInerney's transformed problem corresponds to this constructively interfering modal contribution.

It should be noted that the idea of interference of neutron waves is not new, having been postulated as early as 1964 on the basis of diffusion theory by Perez et al. [60] to explain phenomena observed in wave experiments in subcritical assemblies. More recently, in the transport treatment of polycrystalline materials by Yamagishi [44], interference effects have been seen to arise from interaction of a continuum contribution, due to neutrons with energies below the Bragg cutoff, with the higher energy neutron population. In the present fast nonmultiplying problem we have seen that modal interference is necessary to describe neutron wave propagation in all but purely absorbing materials.

In the same context it is interesting to consider elastic scattering from very heavy nuclei. In this case the energy loss per collision is sufficiently small that wave propagation in such a medium is essentially monochromatic. Thus monoenergetic analyses may be performed such as, for example, those of Ohanian et al. [61] and Paiano and Paiano [62]. In this case, due to the energy-sustaining model of the collision process, space-angle-separable monoenergetic eigenmodes occur which are less attenuated than Σ_t . We realize that in the actual energy-dependent problem an energy loss does occur with each scattering interaction, so that only continuum modes are present; nevertheless these

continuum modes must superimpose in such a way as to yield the almost-separable wave behavior.

The macroscopically elastic scattering kernel model of the above discussion may be written

$$\Sigma_{se}(E', \mu' \rightarrow E, \mu) = \Sigma_{se}(E') K(\mu' \rightarrow \mu) \delta(E - E'). \quad (2.25)$$

This kernel also is noteworthy because it is not bounded. Clearly our discussion of bounded scattering kernels in establishing the resolvent set, $\kappa \notin C$, does not apply and we find spectral contributions do arise for $\kappa \in C$. The model of Eq. (2.25) is discussed in Appendix C, along with several limiting procedures which may be used to attempt to derive the strictly monoenergetic case as the limit of the almost-monoenergetic case.

We conclude the discussion here by observing that another way of viewing the problem of elastic scattering from heavy nuclei is to consider a detector with an energy window ΔE wide enough to detect all elastically scattered neutrons; one should then obtain experimental results which are in accordance with monoenergetic theory. That is, the detector response should show an asymptotic exponential signal decay corresponding to the monoenergetic fundamental mode; this detector response is the physical equivalent of solving for the zeroth moment of the flux rather than the flux itself. In this instance we must agree with Dorning and Thurber [40] who remark in another context that in attempting to correlate theory and experiment one can be misled by

considering only the asymptotic behavior of flux solutions rather than their moments.

Realistic Cross Sections: Nonmonotonic $v\Sigma_t$

In Chapter I analysis was restricted to total cross sections such that $v\Sigma_t$ is monotonic. This was done because the continuum values of κ and all possible E, μ pairs are in one-to-one correspondence for monotonic $v\Sigma_t$, a requirement of the generalized analytic function treatment upon which we rely for completeness results in the separable kernel case. Here we explore briefly the consequences of relaxing the monotonicity condition.

For this case degeneracy of the continuum results. From Eq. (1.19) it is apparent that $\theta(\kappa)$ will assume the same value more than once when $v\Sigma_t$ is not monotonic. This is illustrated in Figure 2.3, where it is evident that for the same value of θ , but different energies, nondegenerate, singly degenerate, and doubly degenerate regions occur. Higher degeneracies may result from more rapidly oscillating cross sections. We exclude the case of constant $v\Sigma_t$, which must be treated separately.

When the continuum is degenerate the coefficient $(a - \mu\kappa)$ in the forward and adjoint eigenvalue equations becomes zero for more than one E, μ pair at each degenerate κ point. Thus in Eq. (2.16) and the corresponding adjoint expression we may make the replacement

$$\begin{aligned} \lambda(\kappa) \delta(a - \mu\kappa) &\rightarrow \sum_{m=1}^M \lambda_m(\kappa) \delta_m(a - \mu\kappa) \\ &\equiv \sum_{m=1}^M \lambda_m(\kappa) \delta(E - E_{\kappa m}) \delta(\mu - \mu_{\kappa m}). \end{aligned} \quad (2.26)$$

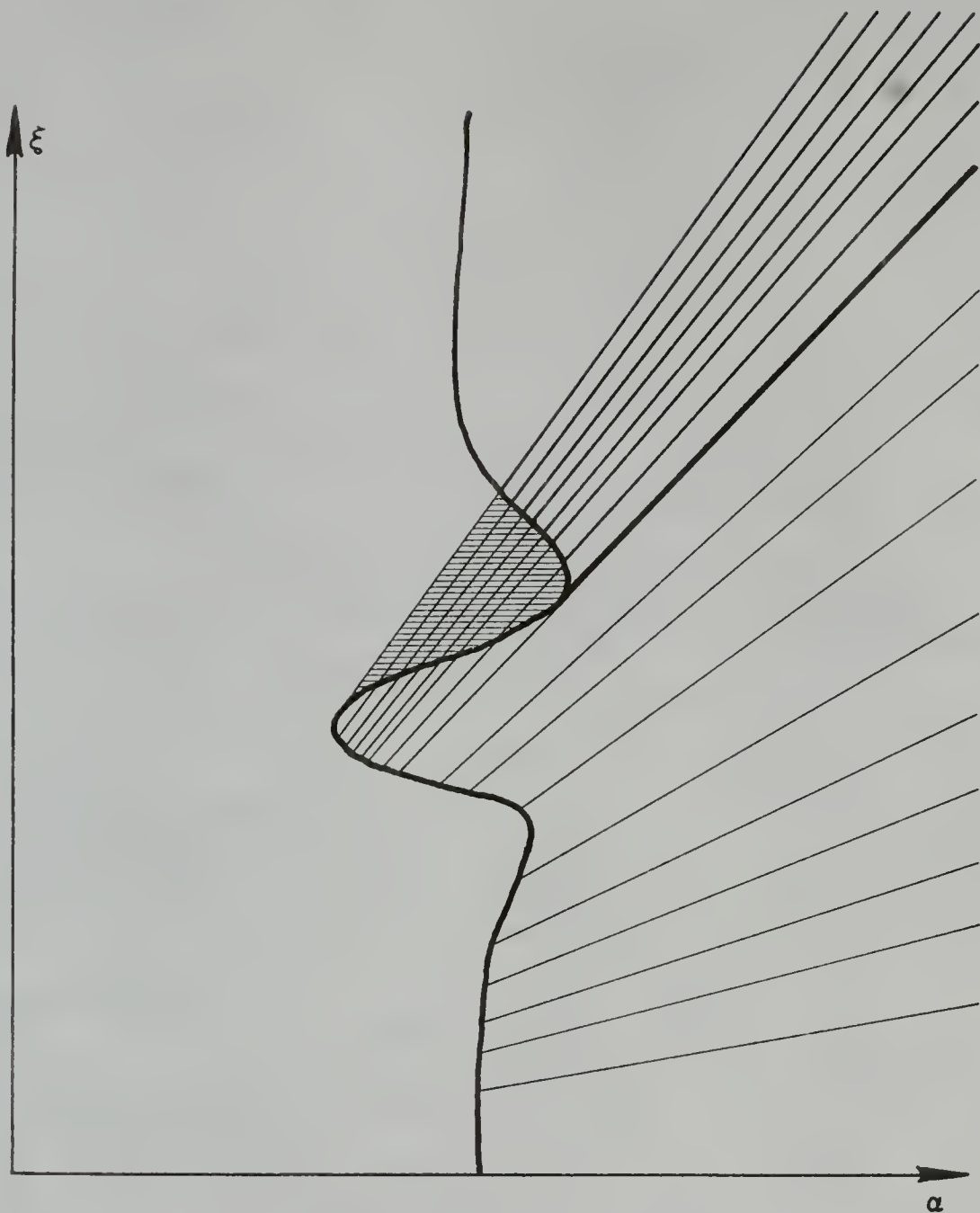


Figure 2.3 Degeneracy of the continuum due to nonmonotonic $v\Sigma_t$.

Thus from Eqs. (2.18) and (2.20) we have

$$F(E, \mu; \kappa) = \sum_{m=1}^M \lambda_m(\kappa) \mathfrak{F} \cdot \delta_m(a - \mu\kappa) \quad (2.27)$$

and

$$F^\dagger(\kappa; E, \mu) = \sum_{m=1}^M \lambda_m^\dagger(\kappa) \mathfrak{F}^\dagger \cdot \delta_m(a - \mu\kappa) \quad (2.28)$$

for an M-degenerate κ . Clearly since there are M arbitrary λ 's, M linearly independent eigenfunctions can be constructed. An obvious choice is to set the λ 's equal to zero for all but one δ_m ; we define the M eigenfunctions

$$F_{SD,m}^\dagger(E, \mu; \kappa) = \lambda_m^\dagger(\kappa) \mathfrak{F}^\dagger \cdot \delta_m(a - \mu\kappa) \quad (2.29)$$

and

$$F_{SD,m}^\dagger(\kappa; E, \mu) = \lambda_m^\dagger(\kappa) \mathfrak{F}^\dagger \cdot \delta_m(a - \mu\kappa) \quad (2.30)$$

which we notice are biorthogonal when the forward eigen-energy is less than the adjoint eigen-energy but are not necessarily biorthogonal otherwise. Also we see from Eq. (2.22) that the forward eigenfunctions will have pole singularities at all eigen-energies $E_{\kappa n}$ less than the

delta-function eigen-energy $E_{\kappa m}$. A similar structure occurs in the adjoint eigenfunctions.

Fast Multiplying Media: Zero Scattering Cross Section

The fast multiplying medium problem best may be approached by first considering Eq. (1.13) with the scattering operator absent. Since the fission interaction kernel is separable, Eq. (1.13) then becomes identical in form to the thermal WBE with separable kernel, Eq. (1.24), which was discussed in detail in the first chapter. Identifying χ with $M(E)$ and $v\Sigma_f(E')$ with $\Sigma_s(E')$, we may write down immediately the results for the nonscattering fast multiplying WBE from Eqs. (1.29), (1.30) and (1.32). Thus we find that the discrete eigenvalues are given by the dispersion law

$$\Lambda(\kappa, \omega) \equiv 1 - \left(v\Sigma_f, \frac{\chi}{a - \mu\kappa} \right) = 0 \quad (2.31)$$

and the corresponding regular eigenfunctions are

$$F(E, \mu; \kappa_j) = \lambda(\kappa_j) \frac{\chi}{a - \mu\kappa_j} \quad \kappa \notin C. \quad (2.32)$$

The singular continuum eigenfunctions are

$$F(E, \mu; \kappa) = \lambda(\kappa) \left[\frac{\chi}{a - \mu\kappa} \frac{v\Sigma_f(E_\kappa)}{\Lambda} + \delta(a - \mu\kappa) \right] \quad \kappa \in C \quad (2.33)$$

Adjoint eigenfunctions, which we obtain for later comparison, are readily found to be

$$F^\dagger(\kappa_j; E, \mu) = \lambda^\dagger(\kappa_j) \frac{v\Sigma_f(E)}{a - \mu\kappa_j} \quad \kappa \notin C \quad (2.34)$$

and

$$F^\dagger(\kappa; E, \mu) = \lambda^\dagger(\kappa) \left[\frac{v\Sigma_f(E)}{a - \mu\kappa} + \frac{\frac{1}{2}\chi(E, \kappa)}{\Lambda} + \delta(a - \mu\kappa) \right] \quad \kappa \in C \quad (2.35)$$

where we have used the definition of $\chi(E)$ from Eq. (1.10). We note that the same dispersion function occurs in both forward and adjoint expressions.

By analogy with the thermal problem we expect a symmetric pair of eigenvalues for moderate frequencies and absorption. We further expect that the set of eigenfunctions of Eqs. (2.32) and (2.33) will have full and half-range completeness properties (although strictly speaking these properties were demonstrated for a symmetrized kernel in the thermal case; a similar symmetrization transformation could be performed in the fast case).

Discrete Eigenfunctions for Fast Multiplying Media

We now turn to solution of the fast WBE with down-scattering, as represented by Eq. (1.13). For $\kappa \notin C$, we may divide by $(a - \mu\kappa)$ and

invert the identity minus the scattering operator (under the conditions which were discussed previously) to obtain

$$F(E, \mu; \kappa) = \mathcal{S} \cdot \frac{\chi}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^{\infty} dE' \nu\Sigma_f(E') F(E', \mu'; \kappa) \quad (2.36)$$

using the inverse operator defined in Eq. (2.18). Taking the scalar product of this equation with $\nu\Sigma_f$, we find that the condition for solutions to exist is that

$$\Lambda(\kappa, \omega) = 1 - \left(\nu\Sigma_f, \mathcal{S} \cdot \frac{\chi}{a - \mu\kappa} \right) = 0 \quad (2.37)$$

which defines the dispersion function and the dispersion law for the discrete eigenvalues κ_j . The expression for the regular eigenfunctions then is

$$F(E, \mu; \kappa_j) = \lambda(\kappa_j) \mathcal{S} \cdot \frac{\chi}{a - \mu\kappa_j} \quad \kappa \notin C. \quad (2.38)$$

This expression may be compared with Eq. (2.32); making use of the Neumann series interpretation of \mathcal{S} , we see that the presence of down-scattering in the problem has resulted in an addition of all iterated collision integrals of the nonscattering eigenfunction (cf. Eq. (2.22)). Thus the discrete eigenfunction consists of the fission spectrum,

weighted by the transport factor $(a - \mu\kappa)^{-1}$ (which is peaked at $\mu = \pm 1$ but not singular, for $\kappa \notin \mathbb{C}$), and smeared down in energy by similarly weighted scattering operators. We will discuss the regular eigenfunctions and the dispersion law in more detail in Chapter IV.

The corresponding adjoint eigenfunctions similarly are found to be

$$F^\dagger(\kappa_j; E, \mu) = \lambda^\dagger(\kappa_j) \mathfrak{S}^\dagger \cdot \frac{\nu \Sigma_f(E)}{a - \mu\kappa_j}. \quad (2.39)$$

It is readily verified that the same dispersion law is obtained here as for the forward problem.

Continuum Eigenfunctions for Fast Multiplying Media

By application to Eq. (1.13) of the arguments used in arriving at Eq. (2.18), we find

$$F(E, \mu; \kappa) = \mathfrak{S} \cdot \frac{\chi}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^\infty dE' \nu \Sigma_f(E') F(E', \mu'; \kappa) + \lambda(\kappa) \mathfrak{S} \cdot \delta(a - \mu\kappa) \quad \kappa \in \mathbb{C} \quad (2.40)$$

which in view of Eq. (2.18) may be written

$$F(E, \mu; \kappa) = \mathfrak{S} \cdot \frac{\chi}{a - \mu\kappa} (\nu \Sigma_f, F) + \lambda(\kappa) F_{SD}(E, \mu; \kappa). \quad (2.41)$$

Eliminating the scalar product term results in the expression

$$F(E, \mu; \kappa) = \lambda(\kappa) \left[\mathfrak{F} \cdot \frac{\chi}{a - \mu\kappa} \frac{(\nu\Sigma_f, F_{SD})}{\Lambda} + F_{SD} \right]$$

$$\kappa \in \mathbb{C} \quad (2.42)$$

for the forward continuum singular eigenfunction, where Λ is defined by Eq. (2.37). The adjoint continuum eigenfunction is

$$F^\dagger(\kappa; E, \mu) = \lambda^\dagger(\kappa) \left[\mathfrak{F}^\dagger \cdot \frac{\nu\Sigma_f}{a - \mu\kappa} \frac{(\chi, F_{SD}^\dagger)}{\Lambda} + F_{SD}^\dagger \right]$$

$$\kappa \in \mathbb{C} \quad (2.43)$$

where in this case $F_{SD}^\dagger \equiv \mathfrak{F}^\dagger \cdot \delta(a - \mu\kappa)$.

Discussion of the Continuum Eigenfunctions

The eigenfunctions represented by Eq. (2.42) have an interesting interpretation much in the same manner as that of Eq. (2.22), and with similar reservations applicable. Making use of Eq. (2.37) for the dispersion function and expanding the inverse in a power series, Eq. (2.42) may be written

$$\frac{F(E, \mu; \kappa)}{\lambda(\kappa)} = \mathfrak{F} \cdot \frac{\chi}{a - \mu\kappa} \left[1 + \left(\nu\Sigma_f, \mathfrak{F} \cdot \frac{\chi}{a - \mu\kappa} \right) + \left(\nu\Sigma_f, \mathfrak{F} \cdot \frac{\chi}{a - \mu\kappa} \right)^2 + \dots \right] \left(\nu\Sigma_f, F_{SD} \right) +$$

$$+ F_{SD}(E, \mu; \kappa) \quad (2.44)$$

Now let us regard $(\nu\Sigma_f, F_{SD})$ as the initial excitation of the fission contribution to the mode. The resulting fission neutrons, after being smeared in energy by scattering, have the energy and angular distribution $\mathcal{S} \cdot \frac{\chi}{a-\mu\kappa}$. The form of the dispersion function expansion suggests that it be interpreted as a modal multiplication due to the sum over all generations of fission neutrons. Thus we see that the continuum mode again may be regarded as streaming-associated, since it consists of two terms which we interpret as follows. The second term is F_{SD} which has been seen to be the down-scattered distribution associated with streaming neutrons having the eigen-energy and eigen-angle. The first term of Eq. (2.44) then may be interpreted as the fission-produced modal flux distribution due to excitation in turn by the scattered term.

This attractive exegesis must be tempered, as in the slowing-down case, by considering the scalar product of the adjoint eigenfunctions, Eq. (2.43), with a monoenergetic source function. We observe first that the source will excite modes with lower eigen-energy, due to the term F_{SD}^\dagger . In addition, modes having eigen-energies both above and below the source energy will be excited due to the fission term $\mathcal{S}^\dagger \cdot \frac{\nu\Sigma_f}{a-\mu\kappa}$.

These results may be compared qualitatively with solutions for the static fast multiplying medium transport problem obtained by Nicolaenko and Zweifel [63] and Nicolaenko [14]. Energy-transform techniques were used to treat fission and elastic scattering with constant cross sections in the former study. Inelastic scattering, the model for which already has been the subject of comment here, was added in the latter. Although detailed comparison again is difficult due to the complex structure of the continuum eigenfunctions, we find consistencies between their Green's

function results and the present work. Specifically, in both studies, Green's function solutions are found to contain both space-separable contributions (which we ascribe to the discrete eigenmode) and nonseparable "slowing-down transients," which are solutions to the slowing-down equation without the fission term, and which were found to be necessary to achieve completeness for the eigenfunctions of the appropriate Boltzmann equation. The correlation with our results is apparent.

Degeneracy of the Continuum

Should further complications seem desirable at this point, consideration may be given to the effect of degeneracies in the continuum upon the above treatment of continuum eigenfunctions. Since the details are straightforward, we simply note that linearly independent sets of eigenfunctions can be obtained; in particular a set corresponding to those of Eqs. (2.29) and (2.30) may be derived by an identical procedure. The eigenfunctions are given by Eqs. (2.42) and (2.43) with the substitution of $F_{SD,m}$ and $F_{SD,m}^\dagger$ for F_{SD} and F_{SD}^\dagger .

The Boltzmann Equation with Isotropic Interaction

Finally, some general consequences of isotropy in the WBE operators will be derived for use in Chapters III and IV. For the isotropic kernel we write

$$K(E', \mu' \rightarrow E, \mu) = K(E' \rightarrow E) \quad (2.45)$$

so that the WBE for $\kappa \notin C$ may be written

$$\begin{aligned} F(E, \mu; \kappa) &= \frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^\infty dE' K(E' \rightarrow E) F(E', \mu'; \kappa) \\ &= \frac{1}{a - \mu\kappa} \int_0^\infty K(E' \rightarrow E) F(E'; \kappa) dE' \end{aligned} \quad (2.46)$$

with the definition

$$F(E; \kappa) \equiv \int_{-1}^1 F(E, \mu; \kappa) d\mu . \quad (2.47)$$

Integrating Eq. (2.46) over μ we obtain

$$F(E; \kappa) = f(E) \int_0^\infty K(E' \rightarrow E) F(E'; \kappa) dE' \quad (2.48)$$

with $f(E)$ defined as

$$f(E) \equiv \int_{-1}^1 \frac{d\mu}{a - \mu\kappa} . \quad (2.49)$$

Upon solution of Eq. (2.48) we then reconstruct the angular flux from

$$F(E, \mu; \kappa) = \frac{f^{-1}(E)}{a - \mu\kappa} F(E; \kappa) . \quad (2.50)$$

For $\kappa \in \mathbb{C}$ the continuum eigenfunction equation becomes

$$F(E, \mu; \kappa) = \frac{1}{a - \mu\kappa} \int_{-1}^1 d\mu' \int_0^\infty dE' K(E' \rightarrow E) F(E', \mu'; \kappa) + \lambda(\kappa) \delta(a - \mu\kappa) . \quad (2.51)$$

Performing integrations over μ we have

$$F(E; \kappa) = f(E) \int_0^\infty K(E' \rightarrow E) F(E'; \kappa) dE' + \lambda(\kappa) \delta(E - E_\kappa) \\ \kappa \in \mathbb{C} . \quad (2.52)$$

CHAPTER III

APPLICATION TO THE TRANSFER MATRIX METHOD

Introduction

In this chapter the analytic results obtained for the WBE will be applied to the transfer matrix formalism of Aronson and Yarmush [64] and Aronson [65-70], making it available in a continuous-energy transport representation. There are two aspects of this technique which make it attractive as a potential method for numerical applications of transport theory. First, it provides a convenient general framework for "problem solving" in terms of certain basic operators (see Aronson [67] for a number of examples). Second, it provides an explicit method for obtaining transmission and reflection operators. As we will see, constructing some of the required operator inverses will be equivalent to determining the half-range orthogonality properties of the WBE eigenfunctions. Although it is not possible in general to do this analytically, numerical inversion techniques certainly may be employed, so that the transfer matrix formalism provides a straightforward approach to this difficult aspect of finite medium problems.

The transfer matrix for slab geometry and its associated eigenvalue problem are derived in Appendix A. Essentially what one must do is find the spectrum and eigenfunctions of a certain operator, $\tilde{\sigma}\tilde{\delta}$, in whatever representation the problem is formulated. From these

eigenfunctions all the relevant transfer matrix operators may be constructed, as well as transmission and reflection operators. Here we will obtain the $\tilde{\sigma}$, $\tilde{\delta}$, and $\tilde{\sigma}\tilde{\delta}$ operators for energy-dependent wave transport with an arbitrary interaction kernel, and then show that for isotropic scattering the eigenfunctions of $\tilde{\sigma}\tilde{\delta}$ may be expressed in terms of WBE eigenfunctions.*

Formal Operator Relationships

The operator relationships required to construct the transfer matrix H for a slab of width τ may be summarized as follows:

$$\tilde{H} = \tilde{S} e^{-\tau\tilde{A}} \tilde{S}^{-1} \quad (3.1)$$

where

$$\tilde{S} = \frac{1}{2} \begin{bmatrix} \tilde{B}_+ & \tilde{B}_- \\ \tilde{B}_- & \tilde{B}_+ \end{bmatrix}$$

$$\tilde{S}^{-1} = \frac{1}{2} \begin{bmatrix} \tilde{C}_+ & \tilde{C}_- \\ \tilde{C}_- & \tilde{C}_+ \end{bmatrix} \quad (3.2)$$

*Definitions used here correspond to those used by Aronson in Ref. [66] and earlier; some quantities differ by a factor of 2 in Refs. [69] and [70].

$$e^{-\tau\tilde{A}} = \begin{bmatrix} e^{-\tau\tilde{\Gamma}} & 0 \\ 0 & e^{+\tau\tilde{\Gamma}} \end{bmatrix} \quad (3.3)$$

and $\tilde{\Gamma}$ is diagonal. To obtain the operators \tilde{B}_{\pm} , \tilde{C}_{\pm} and $\tilde{\Gamma}$ one must first diagonalize an auxiliary operator $\tilde{\sigma}\tilde{\delta}$:

$$\tilde{X}^{-1} \tilde{\sigma}\tilde{\delta} \tilde{X} = \tilde{\Gamma}^2 \quad (3.4)$$

where $\tilde{\Gamma}^2$ is diagonal; then

$$\tilde{B}_{\pm} = \tilde{X} \pm \tilde{\delta} \tilde{X} \tilde{\Gamma}^{-1} \quad (3.5)$$

and

$$\tilde{C}_{\pm} = \tilde{X}^{-1} \pm \tilde{\Gamma}^{-1} \tilde{X}^{-1} \tilde{\sigma} . \quad (3.6)$$

The explicit wave transport representation of these formal relationships will be developed in the following sections.

The Operators $\tilde{\sigma}\tilde{\delta}$, \tilde{X} , and \tilde{X}^{-1}

The operators $\tilde{\sigma}$ and $\tilde{\delta}$ are defined as the sum and difference, respectively, of the operators $\tilde{\alpha}$ and $\tilde{\beta}$, which were found in Appendix A to be

$$\tilde{\alpha} \equiv \int_0^{\infty} dE' \int_0^1 d\mu' \left(\frac{a}{\mu} \delta(E' - E) \delta(\mu' - \mu) - \frac{1}{\mu} K_{BE}(E', \mu' \rightarrow E, \mu) \right) \cdot \quad (3.7)$$

$$\tilde{\beta} \equiv \int_0^{\infty} dE' \int_0^1 d\mu' \left(\frac{1}{\mu} K_{BE}(E', -\mu' \rightarrow E, \mu) \right) \cdot \quad (3.8)$$

where K_{BE} is the kernel of the Boltzmann equation interaction operator (operator A_2 of Chapter I), including scattering and fission. In an abbreviated notation Eqs. (3.7) and (3.8) become

$$\tilde{\alpha} = \frac{a}{\mu} - \frac{\tilde{K}^+}{\mu} \cdot \quad (3.9)$$

$$\tilde{\beta} = \frac{\tilde{K}^-}{\mu} \cdot \quad (3.10)$$

so that

$$\tilde{\sigma} = \tilde{\alpha} + \tilde{\beta} = \frac{a}{\mu} - \frac{1}{\mu} (\tilde{K}^+ - \tilde{K}^-) \cdot \quad (3.11)$$

and

$$\tilde{\delta} = \tilde{\alpha} - \tilde{\beta} = \frac{a}{\mu} - \frac{1}{\mu} (\tilde{K}^+ + \tilde{K}^-) \cdot \quad (3.12)$$

Then their product is

$$\begin{aligned} \tilde{\sigma}\tilde{\delta} &= \frac{a^2}{\mu^2} - \frac{1}{\mu} (\tilde{K}^+ - \tilde{K}^-) \cdot \left(\frac{1}{\mu} (a - \tilde{K}^+ - \tilde{K}^-) \right) \cdot \\ &\quad - \frac{a}{\mu^2} (\tilde{K}^+ + \tilde{K}^-) \cdot \end{aligned} \quad (3.13)$$

in terms of an arbitrary interaction operator. This expression is considerably more simple when $\tilde{K}^+ = \tilde{K}^-$, since the awkward middle term of Eq. (3.13) vanishes. In particular this occurs when all interaction processes are isotropic; we will assume this to be the case throughout the rest of this chapter. We then obtain

$$\begin{aligned} \tilde{\sigma}\tilde{\delta} &= \frac{a^2}{\mu^2} - \frac{2a}{\mu^2} \tilde{K} \\ &= \int_0^\infty dE' \int_0^1 d\mu' \left(\frac{a^2}{\mu^2} \delta(E'-E) \delta(\mu'-\mu) - \frac{2a}{\mu^2} K_{BE}(E' \rightarrow E) \right) \cdot \end{aligned} \quad (3.14)$$

which is the form we will consider here.

We now wish to obtain the operator \tilde{X} and its inverse \tilde{X}^{-1} which will diagonalize $\tilde{\sigma}\tilde{\delta}$ as in Eq. (3.4). This may be done by first finding the spectrum and eigenfunctions of the operator $\tilde{\sigma}\tilde{\delta}$, and then constructing \tilde{X} ; \tilde{X}^{-1} will be constructed in a similar way from eigenfunctions of the adjoint operator. The validity of the diagonalization will of course

require that the sets of eigenfunctions are complete. We write the eigenvalue equation for $\tilde{\sigma}\tilde{\delta}$ as

$$\tilde{\sigma}\tilde{\delta} \cdot \chi(E, \mu; \gamma^2) = \gamma^2 \chi(E, \mu; \gamma^2). \quad (3.15)$$

Now $\tilde{\sigma}\tilde{\delta}$ is an integral operator over E and μ , and we will find that in general it will have an area continuous spectrum as well as a possible discrete spectrum. To clarify the correspondence between the eigenfunction $\chi(E, \mu; \gamma^2)$ and the operator \tilde{X} , let us consider for a moment the simpler case which occurs when $\tilde{\sigma}\tilde{\delta}$ is an ordinary $N \times N$ matrix (as it is, in fact, for the multigroup diffusion representation). Then its spectrum consists of the N discrete eigenvalues γ_i^2 ; $\tilde{\Gamma}^2$ is the diagonal array of the γ_i^2 , and \tilde{X} is the corresponding matrix made up of columns of eigenvectors, $X_{ij} \equiv \chi(E_i; \gamma_j^2)$. The matrix \tilde{X} is then a transformation from the basis generated by the eigenvectors corresponding to the individual γ_j^2 , to the discrete-energy space; similarly, \tilde{X}^{-1} is the inverse transformation.

In the present transport case, the situation is entirely analogous, but the summations over the discrete spectrum must be supplemented by an integral over the continuum values of γ^2 , and summation over the E_i is replaced by integrals over E and μ . Thus $\tilde{\Gamma}^2$ is the diagonal operator consisting of both the discrete eigenvalues of $\tilde{\sigma}\tilde{\delta}$ (if any) and the continuous spectrum, γ^2 . The operator \tilde{X} is made up of "columns" of eigenfunctions $\chi(E, \mu; \gamma^2)$ with γ^2 as the "index"; it will involve both an integral over the continuum and a possible sum over discrete contributions.

In other words, for the continuum, $X(E, \mu; \gamma^2)$ is the kernel of an integral operator over all continuum values of γ^2 .

Assuming that the set of eigenfunctions of $\tilde{\sigma}\tilde{\delta}$ is complete, \tilde{X} may be regarded as a transformation from the basis γ^2 to the basis E, μ , while the operator \tilde{X}^{-1} is the inverse transformation. Writing \tilde{X} formally as

$$\tilde{X} = \int_{\gamma^2} d\gamma^2 X(E, \mu; \gamma^2) \cdot \quad (3.16)$$

(the integral is understood to include the sum over the discrete spectrum, if any) and \tilde{X}^{-1} as

$$\tilde{X}^{-1} = \int_0^\infty dE \int_0^1 d\mu X^{-1}(\gamma^2; E, \mu) \cdot \quad (3.17)$$

the left and right inverse relations become

$$\begin{aligned} \tilde{X}^{-1}\tilde{X} &= \tilde{I} = \int_0^\infty dE \int_0^1 d\mu X^{-1}(\gamma^2; E, \mu) \int_{\gamma^2} d\gamma^2 X(E, \mu; \gamma^2) \cdot \\ &= \int_{\gamma^2} d\gamma^2 \delta(\gamma^2 - \gamma'^2) \cdot \end{aligned} \quad (3.18)$$

and

$$\begin{aligned} \tilde{X}\tilde{X}^{-1} = \tilde{I} &= \int_{\gamma^2} d\gamma^2 X(E', \mu'; \gamma^2) \int_0^\infty dE \int_0^1 d\mu X^{-1}(\gamma^2; E, \mu) \cdot \\ &= \int_0^\infty dE \int_0^1 d\mu \delta(E-E') \delta(\mu-\mu') \cdot \end{aligned} \quad (3.19)$$

where $\delta(\gamma^2 - \gamma'^2)$ is either a Dirac or Kroneker delta for γ^2 in the continuous or discrete spectrum, respectively. The first of these expressions is a biorthogonality relationship for the two functions $X(E, \mu; \gamma^2)$ and $X^{-1}(\gamma^2; E, \mu)$, while the second is a closure requirement over $\mu \in (0, 1]$ (although we will see later that this closure relation is essentially a full-range condition).

Spectrum and Eigenfunctions of $\tilde{\sigma}\tilde{\delta}$

Using the explicit expression for $\tilde{\sigma}\tilde{\delta}$, Eq. (3.14), we may write the eigenvalue equation, Eq. (3.15), as

$$\begin{aligned} \left(\frac{a^2}{\mu^2} - \gamma^2 \right) X &= \left(\frac{a}{\mu} + \gamma \right) \left(\frac{a}{\mu} - \gamma \right) X \\ &= \frac{2a}{\mu^2} \int_0^\infty dE' \int_0^1 d\mu' K_{BE}(E' \rightarrow E) X(E', \mu'; \gamma^2) \cdot \end{aligned} \quad (3.20)$$

Inspection of this equation shows immediately that the coefficients of X on the left-hand side will give rise to a continuum which is identical

to the domain C which we defined in connection with the WBE; that is, when $\gamma \in C$ it is also in the continuous spectrum of $\tilde{\sigma}\tilde{\delta}$. Further, we now may apply the singular eigenfunction technique to obtain an expression for the continuum X eigenfunctions. Noting that

$$\left(\frac{a}{\mu} + \gamma\right) \left(\frac{a}{\mu} - \gamma\right) \frac{\mu^2}{2a} = \left(\frac{1}{a-\mu\gamma} + \frac{1}{a+\mu\gamma}\right)^{-1} \quad (3.21)$$

we find that for $\gamma \in C$

$$X = \left(\frac{1}{a-\mu\gamma} + \frac{1}{a+\mu\gamma}\right) \int_0^{\infty} dE' \int_0^1 d\mu' K_{BE}(E' \rightarrow E) X(E', \mu'; \gamma^2) + \lambda(\gamma) \delta(a-\mu\gamma) \quad (3.22)$$

where we explicitly consider only γ 's contained in the half of C which is in the first quadrant of the spectral plane; including the other half of the domain C gives redundant results. For $\gamma \notin C$ we have simply

$$X = \left(\frac{-1}{a-\mu\gamma} + \frac{1}{a+\mu\gamma}\right) \int_0^{\infty} dE' \int_0^1 d\mu' K_{BE}(E' \rightarrow E) X(E', \mu'; \gamma^2) \quad (3.23)$$

for the rest of the spectrum of $\tilde{\sigma}\tilde{\delta}$. Now since the stipulation has been made that K_{BE} is isotropic, Eqs. (3.22) and (3.23) may be integrated immediately over μ to give

$$X(E; \gamma^2) = f(E) \int_0^\infty dE' K_{BE}(E' \rightarrow E) X(E'; \gamma^2) + \lambda(\gamma) \delta(E - E_\gamma), \quad \gamma \in C \quad (3.24)$$

$$X(E; \gamma^2) = f(E) \int_0^\infty dE' K_{BE}(E' \rightarrow E) X(E'; \gamma^2), \quad \gamma \notin C \quad (3.25)$$

where $f(E)$ is the same function defined in Eq. (2.49). But these equations are the eigenvalue equations for the WBE with an isotropic kernel. Thus we have the following results:

- (a) The spectrum of the isotropic $\tilde{\sigma}\tilde{\delta}$ operator is identical to the spectrum of the related Boltzmann operator.
- (b) The μ -integrated eigenfunctions of the two operators are identical.

That is, identifying γ with κ ,

$$X(E; \gamma^2) = F(E; \kappa) \quad (3.26)$$

so

$$\begin{aligned} & \int_0^\infty dE' \int_0^1 d\mu' K_{BE}(E' \rightarrow E) X(E', \mu'; \gamma^2) = \\ & = \int_0^\infty dE' K_{BE}(E' \rightarrow E) X(E'; \gamma^2) \\ & = \int_0^\infty dE' K_{BE}(E' \rightarrow E) F(E'; \kappa) \end{aligned}$$

$$= \int_0^{\infty} dE' \int_{-1}^1 d\mu' K_{BE}(E' \rightarrow E) F(E', \mu'; \kappa). \quad (3.27)$$

Using this identity in Eqs. (3.22) and (3.23) and comparing with Eqs. (2.46) and (2.52) for eigenfunctions of the WBE, we find that for an isotropic K_{BE}

$$\chi(E, \mu; \kappa^2) = F(E, \mu; \kappa) + F(E, \mu; -\kappa). \quad (3.28)$$

The Inverse Operator $\tilde{\chi}^{-1}$

To obtain the inverse operator $\tilde{\chi}^{-1}$ analytically the most obvious approach is to construct it from the eigenfunctions of the operator adjoint to $\tilde{\sigma}\tilde{\delta}$; it then should have the required biorthogonality properties of Eq. (3.18). Referring to Eq. (3.19) we see that the appropriate scalar product is

$$(\phi, \psi) \equiv \int_0^{\infty} dE \int_0^1 d\mu \phi(E, \mu) \psi(E, \mu) \quad (3.29)$$

which leads to the adjoint isotropic eigenvalue equation

$$\left(\frac{a^2}{\mu^2} - \kappa^2 \right) \chi^{-1}(\kappa^2; E, \mu) = 2 \int_0^{\infty} dE' \int_0^1 d\mu' \frac{a(E')}{\mu'^2} K_{BE}(E \rightarrow E') \chi^{-1}(\kappa^2; E', \mu'). \quad (3.30)$$

Defining the function

$$X^\dagger(\kappa^2; E, \mu) = \frac{a}{\mu^2} X^{-1}(\kappa^2; E, \mu) \quad (3.31)$$

and substituting in Eq. (3.30),

$$\left(\frac{a^2}{\mu^2} - \kappa^2 \right) X^\dagger(\kappa^2; E, \mu) = \frac{2a}{\mu^2} \int_0^\infty dE' \int_0^1 d\mu' K_{BE}(E \rightarrow E') X^\dagger(\kappa^2; E', \mu') \quad (3.32)$$

where $K_{BE}(E \rightarrow E')$ is the kernel of the adjoint WBE considered in Chapter II. By duplicating the development of Eq. (3.20) we have immediately

$$X^\dagger(\kappa^2; E) = F^\dagger(\kappa; E) \quad (3.33)$$

and

$$X^\dagger(\kappa^2; E, \mu) = F^\dagger(\kappa; E, \mu) + F^\dagger(-\kappa; E, \mu) \quad (3.34)$$

making use of the eigenfunctions of the adjoint WBE from Chapter II.

Then $X^{-1}(\kappa^2; E, \mu)$ is given by Eq. (3.31).

Diagonalization Operators

These results now may be used to obtain expressions for the operators \tilde{B}_\pm and \tilde{C}_\pm which diagonalize the transfer matrix itself (Eqs. (3.1) - (3.3)). From Eqs. (3.5) and (3.6)

$$\tilde{B}_{\pm} = \tilde{X} \pm \tilde{\delta} \tilde{X} \tilde{\Gamma}^{-1} \equiv \tilde{X} \pm \tilde{\xi} \quad (3.35)$$

and

$$\tilde{C}_{\pm} = \tilde{X}^{-1} \pm \tilde{\Gamma}^{-1} \tilde{X}^{-1} \tilde{\sigma} \equiv \tilde{X}^{-1} \pm \tilde{\xi}^{-1} . \quad (3.36)$$

Since $\tilde{\Gamma}$ is diagonal, elements of $\tilde{\xi}$ may be written

$$\begin{aligned} \xi(E, \mu; \kappa) &= \frac{1}{\kappa} \int_0^{\infty} dE' \int_0^1 d\mu' \left(\frac{a(E')}{\mu'} \delta(E' - E) \delta(\mu' - \mu) \right. \\ &\quad \left. - \frac{2}{\mu} K_{BE}(E' \rightarrow E) \right) X(E', \mu; \kappa^2) \\ &= \frac{\mu\kappa}{a} X(E, \mu; \kappa^2) \end{aligned} \quad (3.37)$$

making use of Eqs. (3.12) and (3.20). Then

$$B_{\pm}(E, \mu; \kappa) = \frac{a \pm \mu\kappa}{a} X(E, \mu; \kappa^2) . \quad (3.38)$$

For isotropic K_{BE} we note that

$$(a - \mu\kappa) F(E, \mu; \kappa) = (a + \mu\kappa) F(E, \mu; -\kappa) \quad (3.39)$$

so that from Eq. (3.28)

$$B_{\pm}(E, \mu; \kappa) = 2F(E, \mu; \pm\kappa). \quad (3.40)$$

Similarly $\tilde{\xi}^{-1}$ is

$$\tilde{\xi}^{-1} = \int_{\kappa^2} d\kappa' \frac{1}{\kappa'} \delta(\kappa' - \kappa) \int_0^{\infty} dE \int_0^1 d\mu X^{-1}(\kappa'^2; E, \mu) \int_0^{\infty} dE' \int_0^1 d\mu' \frac{a(E')}{\mu'} \delta(E' - E) \delta(\mu' - \mu). \quad (3.41)$$

so that

$$\xi^{-1}(\kappa; E, \mu) = \frac{a}{\mu\kappa} X^{-1}(\kappa^2; E, \mu) \quad (3.42)$$

and

$$C_{\pm}(\kappa; E, \mu) = \frac{\mu}{a\kappa} (a \pm \mu\kappa) X^{\dagger} = \pm \frac{2\mu}{\kappa} F^{\dagger}(\pm\kappa; E, \mu) \quad (3.43)$$

making use of Eqs. (3.31) and (3.34), and Eq. (3.39) which also applies to F^{\dagger} .

Full-Range Orthogonality and Completeness

At this point \tilde{B}_{\pm} and \tilde{C}_{\pm} are still determined only to within a normalization function of κ . The normalization relationship may be obtained by considering the operators \tilde{S} and \tilde{S}^{-1} of Eq. (3.2). Substitution of Eqs. (3.38) and (3.43) for \tilde{B}_{\pm} and \tilde{C}_{\pm} into the left inverse expressions $\tilde{S}^{-1}\tilde{S} = \tilde{I}$ yields the appropriate expression, which, with a little manipulation, is also found (as for the monoenergetic case [68])

to be a whole-range biorthogonality relation for the WBE eigenfunctions F and F^\dagger . Similarly, the right inverse equation (which in view of Eq. (3.1) expresses explicitly the physical requirement that as the slab width τ is decreased to zero, the transfer matrix must reduce to the identity) $\tilde{S}\tilde{S}^{-1} = I$ is found to be a whole-range closure expression for F and F^\dagger . Thus we see that the validity of the diagonalization in Eqs. (3.1) - (3.3) depends on the full-range biorthogonality and completeness of the WBE eigenfunctions, properties which may be established in the context of the WBE itself.

Half-Range Orthogonality and Completeness

The entire transfer matrix \tilde{H} now has been obtained without explicit application of any half-range conditions. (It was not necessary to solve Eqs. (3.18) and (3.19) for the inverse of \tilde{X} .) However, we recall that the transfer matrix relates the angular flux over $\mu \in [-1, 1]$ at one slab surface to the corresponding flux at the other. It is apparent that use of the full transfer matrix is completely equivalent to applying full-range boundary conditions at one interface to an infinite-medium eigenfunction expansion of the flux, which, of course, completely determines the flux elsewhere within the slab, and in particular at the opposite surface. In situations where only incident fluxes are known at interfaces, the transmission and reflection operators \tilde{T} and \tilde{R} are more appropriate to the problem. It is in constructing these operators that half-range conditions will appear.

The transfer matrix formalism provides expressions for \tilde{T} and \tilde{R} in terms of the diagonalization operators \tilde{B}_\pm and \tilde{C}_\pm (Eqs. (A.63) through

(A.66)), all of which are defined for $\mu \in (0,1]$. However, inverses of the operators \tilde{B}_{\pm} and \tilde{C}_{\pm} occur explicitly, and must be evaluated for the interval $(0,1]$ if one is to compute \tilde{T} and \tilde{R} . Thus, for \tilde{B}_{\pm} , we have the inverse relationships, using Eq. (3.40),

$$2 \int_0^{\infty} dE \int_0^1 d\mu B_{\pm}^{-1}(\kappa; E, \mu) F(E, \mu; \pm\kappa) = \delta(\kappa' - \kappa) \quad (3.44)$$

and

$$2 \int_{\kappa^2} d\kappa F(E, \mu; \pm\kappa) B_{\pm}^{-1}(\kappa; E', \mu') = \delta(E' - E) \delta(\mu' - \mu). \quad (3.45)$$

Solving the singular integral equation, Eq. (3.44), for B_{\pm}^{-1} is equivalent to obtaining the weight function $W(E, \mu)$ and normalization $N(\kappa)$ for half-range biorthogonality of F and F^{\dagger} , since if they are complete on the half-range we identify

$$2B_{\pm}^{-1}(\kappa; E, \mu) = N(\kappa)W(E, \mu)F^{\dagger}(\pm\kappa; E, \mu) \quad (3.46)$$

so that Eq. (3.45) becomes a closure relation for the WBE eigenfunctions.

It was pointed out previously that for most realistic interaction models analytic solutions of Eqs. (3.44) and (3.45) are not likely to be readily forthcoming, and consequently the transmission and reflection operators must be constructed without analytic expressions for the required inverses. (In this respect the invariant imbedding method is an alternative, as it provides a completely different formulation for

\tilde{R} and \tilde{T} . See Pfeiffer and Shapiro [71] for a review of the various approaches to transmission and reflection, and Mockel [54] for an example of application of both transfer matrix and invariant imbedding methods to thermal neutron wave propagation.) Nevertheless, supposing that some approximate numerical representation has been found for the WBE eigenfunctions, one can always invert the diagonalization operators numerically, which we have seen to be exactly equivalent to numerically determining half-range normalization of the WBE eigenfunctions. After the numerical inversion is performed, \tilde{R} and \tilde{T} also may be calculated numerically.

Application to Fast Neutron Wave Propagation

We have seen that for isotropic interactions all the essential operators required to apply the transfer matrix technique may be constructed from solutions of the WBE eigenfunction problem. Further, requirements for half- and full-range closure and biorthogonality of these eigenfunctions are implicit in the formalism. These results and in particular Eqs. (3.28), (3.34), (3.40), and (3.43) extend Aronson's static monoenergetic work [65-70], and are quite general with respect to the energy-dependence of the kernel.

It is interesting to note that relationships between transfer matrix and Boltzmann equation eigenfunctions, analogous to these equations, have been obtained for arbitrary anisotropic scattering and for azimuthally dependent problems in the monoenergetic case [69]. While there is no new physics per se in the transfer matrix approach beyond that contained in the WBE, and thus one expects a direct interrelationship

between the two eigenvalue problems [68], it remains to be seen whether the simple form of Eqs. (3.28) and (3.34) will hold for energy-dependent formulations with anisotropic scattering. It should be stressed that since no stipulations other than scattering isotropy have been made with respect to the interaction kernel in this chapter, the results obtained here apply equally to fast and thermal regions, with or without fission, etc. Furthermore, the form of the term $a(E,\omega)$, which we have taken to be $\Sigma_t + \frac{i\omega}{v}$, does not enter explicitly and therefore generalization is immediate to finite transverse dimensions through introduction of a transverse buckling. Of course the static case $\omega = 0$ is included.

Thus the equivalence of the continuous energy transfer matrix and WBE eigenfunction approaches for isotropic interactions is quite apparent, so that we may regard the transfer matrix method as a possibly convenient framework for application of the WBE analysis. In this sense we now have in the results of this chapter a complete treatment of the analytic basis of the isotropic scattering energy-dependent transfer matrix. Application to fast neutron wave and pulse propagation thus is a matter of finding suitable means of implementing the formal results obtained in Chapter II, using the basic relationships developed here.

CHAPTER IV

APPLICATION TO DISPERSION LAW AND DISCRETE EIGENFUNCTION CALCULATIONS

Introduction

Expressions for the spectrum and eigenfunctions of the fast multiplying WBE were derived in Chapter II. Emphasis there was placed on application of the singular eigenfunction technique to obtain formal expressions for the continuum eigenfunctions. In this chapter we will consider the mathematically more straightforward topic of the discrete spectrum and regular eigenfunctions of the wave transport operator.

This subject now is quite thoroughly understood in principle for the separable fission kernel model; Travelli [16] has presented an essentially complete transport multigroup numerical treatment of the fast wave slab-geometry eigenvalue problem which takes into account scattering anisotropy, through a P_N expansion, and delayed neutrons. However, apart from Travelli's work and the present investigation [72], this author is not aware of any other numerical fast neutron wave results which have been reported. It is surprising indeed, in view of the apparent timeliness of fast space-dependent kinetics studies, that use is not being made of tools such as these to investigate neutron disturbance propagation in detail.

In this chapter an interrelationship between the dispersion function and regular eigenfunctions is made explicit, and some properties of the

dispersion law are noted. An application of these relationships is made to the dispersion law for multiplying media with isotropic elastic slowing-down and inelastic scattering. Numerical results are presented for the case of one elastically scattering species.

The Dispersion Function and Discrete Eigenfunctions

The dispersion law concept in the context of neutron wave propagation originally was introduced by Moore [73] as a relationship between wave frequency and complex wave length; subsequently this concept was rather broadly generalized [8-10], as discussed in Chapter I. We have seen here, in an exact transport treatment of the fast neutron wave problem, how the dispersion function occurs in the structure of solutions in multiplying media, as indeed it does for all energy-regenerative media, as a result of the presence of a Fredholm integral operator. We now will proceed to formulate the discrete mode eigenvalue problem for a separable fission kernel in a way which both appeals to intuition and suggests a method for computing the dispersion law.

The dispersion functions for fast multiplying media with a separable kernel were given by Eqs. (2.31) and (2.37) for the cases when downscattering is absent and present respectively. These expressions may be summarized by

$$\Lambda = 1 - (v\Sigma_f, G) \quad (4.1)$$

where

$$G(E, \mu; \kappa) = \beta \cdot \frac{\chi}{a - \mu\kappa} \quad (4.2)$$

with \mathcal{S} defined from Eqs. (2.17) and (2.18); when scattering is ignored $\mathcal{S} = I$. The operator \mathcal{S} in Eq. (4.2) may be inverted and the equation multiplied by $(a - \mu\kappa)$ to give

$$(a - \mu\kappa)G(E, \mu; \kappa) - \int_{-1}^1 d\mu' \int_E^\infty dE' \Sigma_s(E', \mu' \rightarrow E, \mu)G(E, \mu; \kappa) = \chi. \quad (4.3)$$

Thus the function $G(E, \mu; \kappa)$ is the solution to a pure slowing-down WBE with the normalized fission spectrum χ as a source, corresponding (cf. Eq. (1.4)) to the space- and time-dependent source $\chi e^{i\omega t} e^{-\kappa x}$. From Eq. (4.1) we see that κ is an eigenvalue when $G(E, \mu; \kappa)$ satisfies $(\nu\Sigma_f, G) = 1$; in that case, comparing Eq. (4.2) to Eq. (2.38), we see that G is an eigenfunction of the total WBE with the particular normalization $\lambda(\kappa) = 1$. The term Λ^{-1} already has been interpreted in the discussion of the form of the multiplying medium continuum eigenfunctions as a modal multiplication factor; here we may regard the dispersion law as a modal prompt criticality condition which determines the value of κ for which a solution to the homogeneous eigenfunction equation will exist.

An analogous interpretation of the dispersion law for the die-away experiment in fast multiplying systems has been given by Moore [8] and Dorning [41], generalizing the work of Storrer and Stiévenart [74] who arrived at an expression for the fast pulsed neutron dispersion law by considering successive generations of fission neutrons. The particularly simple forms above and in the pulsed neutron case for the dispersion function and eigenfunction in terms of $\nu\Sigma_f$ and χ are a direct consequence of the separable form of the fission kernel [8,41,74]. We will see how these results generalize for a degenerate fission kernel.

Algorithms for Evaluating the Discrete Spectrum and Eigenfunctions

Two different numerical approaches to the solution of the eigenvalue problem are suggested by the form of the WBE and Eqs. (4.1)-(4.3). Travelli has employed both [16,30], having derived the techniques by means of computational considerations. The first method is a direct numerical solution of the P_N multigroup representation of Eq. (1.13) for $\kappa \notin \mathbb{C}$; other than the requirement for complex arithmetic this approach is straightforward [30]. An alternative procedure is suggested by Eq. (4.3). In form it is a familiar slowing-down equation, for which solution techniques are well established. The function $G(E, \mu; \kappa)$ is obtained readily for a particular value of κ by solution of Eq. (4.3); the dispersion function Λ may be evaluated by Eq. (4.1). Zeroes of Λ for a particular ω then may be found by application of a complex Newton-Raphson procedure. This procedure has the advantage of not requiring solution of a matrix eigenvalue problem, which can become prohibitively lengthy for the large numbers of energy groups needed to achieve accuracy in fast medium problems [16].

The Newton-Raphson procedure can be expedited by computing $\frac{\partial \Lambda}{\partial \kappa}$ by the following scheme [73]. Differentiating Eq. (4.1) yields

$$\frac{\partial \Lambda}{\partial \kappa} = - (\nu \Sigma_f, \frac{\partial G}{\partial \kappa}) \quad (4.4)$$

and from Eq. (4.3),

$$(a - \mu \kappa) \frac{\partial G}{\partial \kappa} - \int_{-1}^1 d\mu' \int_E^{\infty} dE' \Sigma_s(E', \mu' \rightarrow E, \mu) \frac{\partial G}{\partial \kappa} = \mu G \quad (4.5)$$

which is a slowing-down equation with μG as a source. Solution of Eqs. (4.3) and (4.5) can be carried out in parallel.

Extension to Degenerate Kernels

Only a slight additional effort is required to formulate the eigenvalue problem for a degenerate Fredholm kernel (e.g., multiple fissioning species). Following our development for the separable kernel model we obtain instead of Eq. (2.36)

$$\begin{aligned}
 F(E, \mu; \kappa) &= \sum_{m=1}^M \beta \cdot \frac{\chi^{(m)}}{a - \mu \kappa} \int_{-1}^1 d\mu' \int_0^{\infty} dE' \nu \Sigma_f^{(m)} F(E', \mu'; \kappa) \\
 &\equiv \sum_{m=1}^M G^{(m)}(y^{(m)}, F)
 \end{aligned} \tag{4.6}$$

using obvious notation for an M-term degenerate fission kernel.

Reducing this to the matrix equation

$$(y^{(n)}, F) = \sum_{m=1}^M (y^{(n)}, G^{(m)}) (y^{(m)}, F) \tag{4.7}$$

in the usual way, we find the condition for existence of a solution is the dispersion law

$$\text{Det} \left[I - [(y^{(n)}, G^{(m)})] \right] = \Lambda = 0 \tag{4.8}$$

where the quantity in brackets is the M x M matrix having elements

$$(y^{(n)}, G^{(m)}) = \left[\nu \Sigma_f^{(n)}, \beta \cdot \frac{\chi^{(m)}}{a - \mu \kappa} \right]. \tag{4.9}$$

It is interesting to note that the $G^{(m)}$ are solutions to M slowing-down problems like Eq. (4.3), each with the same scattering operator but with the source energy distribution $\chi^{(m)}$ characteristic of the m^{th} species. Eq. (4.8) is more complicated than previous expressions for the dispersion function, but evidently we may retain our interpretation of Λ^{-1} as a modal multiplication factor; we notice that all combinations of fission of the n^{th} species due to down-scattered neutrons from the m^{th} species occur.

Values of κ which satisfy Eq. (4.8) may be determined by straightforward extension of the Newton-Raphson scheme discussed above. The eigenfunction $F(E, \mu; \kappa)$ then may be reconstructed by means of Eq. (4.6); the coefficients $(y^{(m)}, F)$ are the elements of the eigenvectors of the matrix equation, Eq. (4.7), and the functions $G^{(m)}$ will have been evaluated in satisfying the dispersion law. Thus we have achieved a general extension of the separable kernel analysis to the discrete spectrum and eigenfunctions of the WBE with slowing-down and a degenerate fission (or thermalization) kernel.

As a postscript to the above discussion, we note that the entire procedure is identical in the case of the adjoint eigenfunctions, with the obvious transpose and interchange of $\chi^{(m)}$ and $v\Sigma_f^{(n)}$, and with use of \mathcal{G}^\dagger rather than \mathcal{G} . Further, it is easy to show that

$$(y^{(n)}, G^{(m)}) \equiv (v\Sigma_f^{(n)}, G^{(m)}) = (G^\dagger{}^{(n)}, \chi^{(m)}), \quad (4.10)$$

where

$$G^\dagger \equiv \mathcal{G}^\dagger \cdot \frac{v\Sigma_f}{a - \mu\kappa} \quad (4.11)$$

so that should one wish to construct forward and adjoint solutions simultaneously it is necessary to solve Eq. (4.8) only once.

Isotropic Elastic and Inelastic Scattering

The slowing-down equations encountered in the previous sections are solved readily by any of a number of methods available from the fast reactor literature; see, for example, the review of Okrent et al. [75]. To illustrate the method described above we will develop the expressions for a continuous slowing down [76,77] model, with the addition of a simple inelastic scattering model as well.

For isotropic scattering, Eq. (4.3) may be written

$$G(E;\kappa) - f(E) \int_E^{\infty} \frac{1}{2} \Sigma_S(E' \rightarrow E) G(E';\kappa) dE' = f(E)\chi \quad (4.12)$$

using Eq. (2.49) for $f(E)$; cf. Eqs. (2.48) and (2.52). Differentiating with respect to κ , we obtain

$$\frac{\partial G(E;\kappa)}{\partial \kappa} - f(E) \int_E^{\infty} \frac{1}{2} \Sigma_S(E' \rightarrow E) \frac{\partial G}{\partial \kappa} dE' = \frac{G(E;\kappa)}{f(E)} \frac{\partial f}{\partial \kappa} \quad (4.13)$$

which is the isotropic equivalent of Eq. (4.5). (The μ -dependent eigenfunction can be constructed from the μ -integrated form by using Eq. (2.50).)

For isotropic inelastic scattering from M species and inelastic scattering from N levels with a constant energy loss ΔE_n per interaction we have, in standard notation, the interaction operator

$$\begin{aligned}
\int_E^\infty dE' \Sigma_S(E' \rightarrow E) \cdot &= \sum_{m=1}^{NE} \int_E^{E/\alpha_m} dE' \frac{\Sigma_{se}^{(m)}(E')}{E'(1-\alpha_m)} \cdot + \\
&+ \sum_{n=1}^{NI} \int_E^\infty dE' \Sigma_{si}^{(n)}(E') \delta(E-E'+\Delta E_n) \cdot . \quad (4.14)
\end{aligned}$$

Defining

$$H(E; \kappa) = \frac{G(E; \kappa)}{f(E)} \quad (4.15)$$

and using Eq. (4.14), we find

$$\begin{aligned}
H(E; \kappa) &= \sum_{m=1}^{NE} \int_E^{E/\alpha_m} \frac{1}{2} \frac{\Sigma_{se}^{(m)}(E')}{E'(1-\alpha_m)} f(E') H(E') dE' + \\
&+ \sum_{n=1}^{NI} \frac{1}{2} \Sigma_{si}^{(n)}(E+\Delta E_n) f(E+\Delta E_n) H(E+\Delta E_n) + \chi \quad (4.16)
\end{aligned}$$

and a similar equation for (4.13). Eq. (4.16) is solved most conveniently by converting to the lethargy variable $u = \ln \frac{E_0}{E}$, and differentiating with respect to u . The resulting equation

$$\begin{aligned}
\frac{\partial H(u; \kappa)}{\partial u} &= \frac{\partial}{\partial u} \left(\frac{1}{2} \chi(u) e^u \right) + \frac{1}{2} \sum_{m=1}^{NE} \left(\frac{\Sigma_{se}^{(m)}(u)}{1-\alpha_m} f(u) H(u) \Big|_{u+1n\alpha_m}^u \right) + \\
&+ \frac{1}{2} \sum_{n=1}^{NI} \frac{E(u)}{E(u_n)} \frac{\partial}{\partial u_n} [\Sigma_{si}^{(n)}(u_n) f(u_n) H(u_n) E(u_n)] \quad (4.17)
\end{aligned}$$

is readily integrated numerically, beginning with zero lethargy located above the maximum fission spectrum energy, e.g., 10 MeV. In Eq. (4.17) we have defined

$$H(u;\kappa) = \frac{G(u;\kappa)e^u}{f(u)}. \quad (4.18)$$

Illustrative Results: Dispersion Law and Eigenfunctions for Single Scattering Species

This method of solution was applied to Eq. (4.17) and a related equation for $\frac{\partial G}{\partial \kappa}$, for a one-term elastic scattering kernel. These expressions were implemented as explicit difference equations. The Newton-Raphson method employing Eqs. (4.1) and (4.4) was used to find zeroes of the dispersion function. All cross sections were taken to be constant. Note that with constant total cross section the boundary of the continuum does not change with frequency.

Two computed dispersion laws are shown in Figure 4.1, illustrating the effect of different values for multiplication. Values of κ and ω are expressed in units of Σ_t . Computations were based on scattering from a nuclide of mass 230. A Maxwellian fission distribution having an average neutron energy of 1.98 MeV was used. Here, as in the work of Travelli [16], only one discrete mode per frequency was found, in accordance with the no-scattering case (i.e., by analogy with the thermal separable kernel results). As would be expected the less strongly multiplying eigenfunctions are in general more rapidly attenuated.

Eigenfunctions corresponding to individual points on the dispersion curves may be reconstructed from the computed functions $H(u)$ using

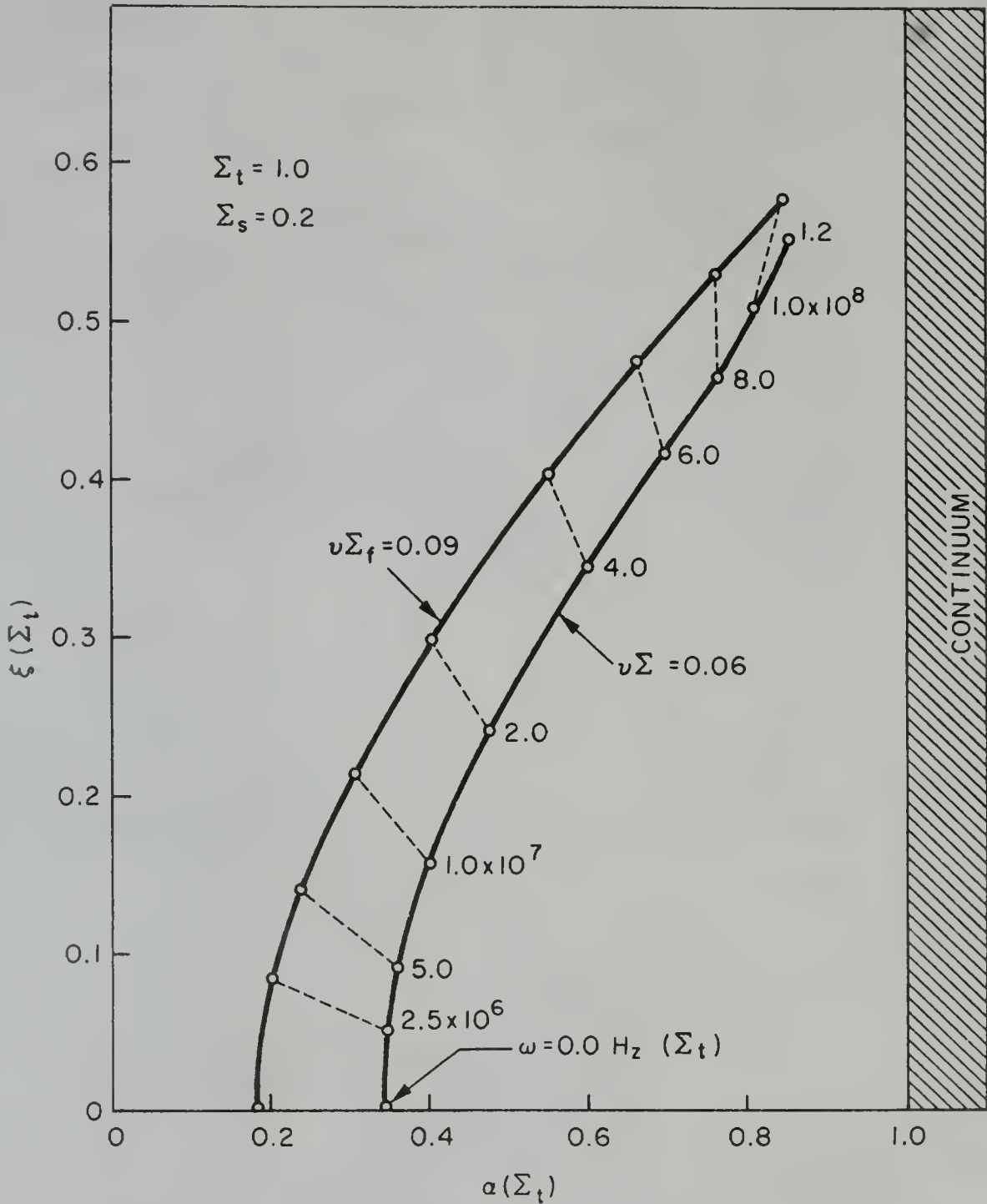


Figure 4.1 Dispersion laws for constant cross-section, elastic scattering model.

Eq. (4.18). With arbitrary normalization constant λ the isotropic eigenfunction $F(u;\kappa)$ is

$$\begin{aligned} F(u;\kappa) &= \lambda G(u;\kappa) \\ &= \lambda H(u;\kappa) f(u) e^{-u} . \end{aligned} \quad (4.19)$$

Zero frequency eigenfunctions, which are real-valued, are shown in Figure 4.2, corresponding to the zero frequency points in Figure 4.1. The eigenfunctions are normalized to coincide with the fission spectrum $\chi(u)$ at lower energies; the effect of down-scattering is noticeable at higher energies.

Amplitudes and phases for the complex-valued eigenfunctions are shown in Figures 4.3 and 4.4. Amplitudes have been plotted with different normalization to separate the curves. These and subsequent data refer to the $\nu\Sigma_f = 0.09$ dispersion law. For relatively moderate frequencies, $\frac{\omega}{\Sigma_t} < 1 \times 10^7$, there is little departure from the zero-frequency energy distribution for energies above about 0.2 MeV. With frequency increasing through the midrange of the dispersion law it appears that neutrons of lower energies experience increasing difficulty keeping pace with the wave. At $\frac{\omega}{\Sigma_t} = 4 \times 10^7$, oscillations in the phase occur at about 0.5 MeV accompanied by some noticeable structure in the amplitude. As frequency increases beyond this value severe phase lagging occurs for lower energy neutrons; Figure 4.5 shows this effect, with phase and amplitude values superimposed. It is interesting that the amplitude maximum occurs in a region of rapidly varying phase. As frequency increases toward the continuum, the eigenfunction becomes increasingly peaked, as shown in Figure 4.6. This bunching of the

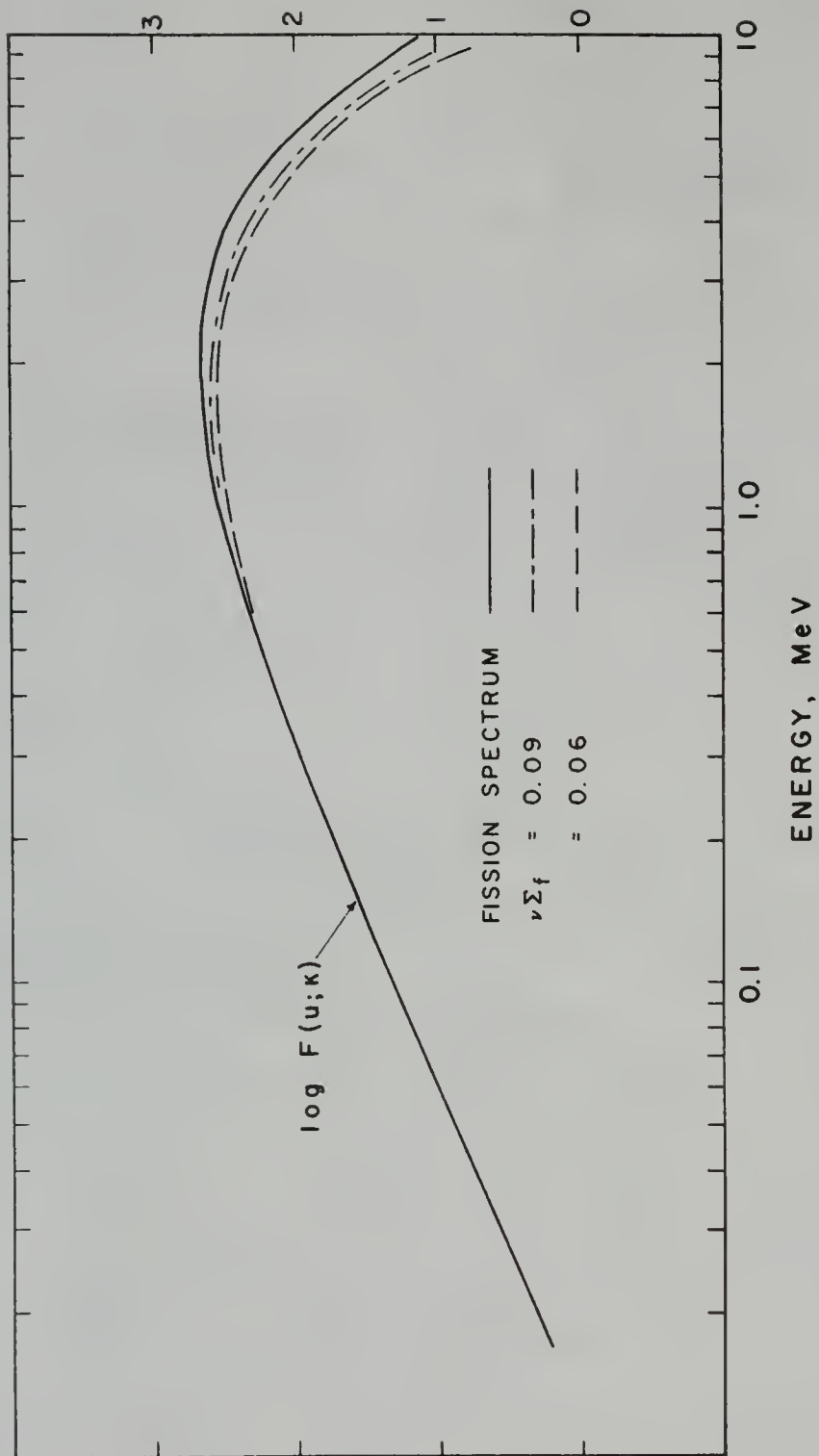


Figure 4.2 Zero frequency eigenfunction energy spectra.

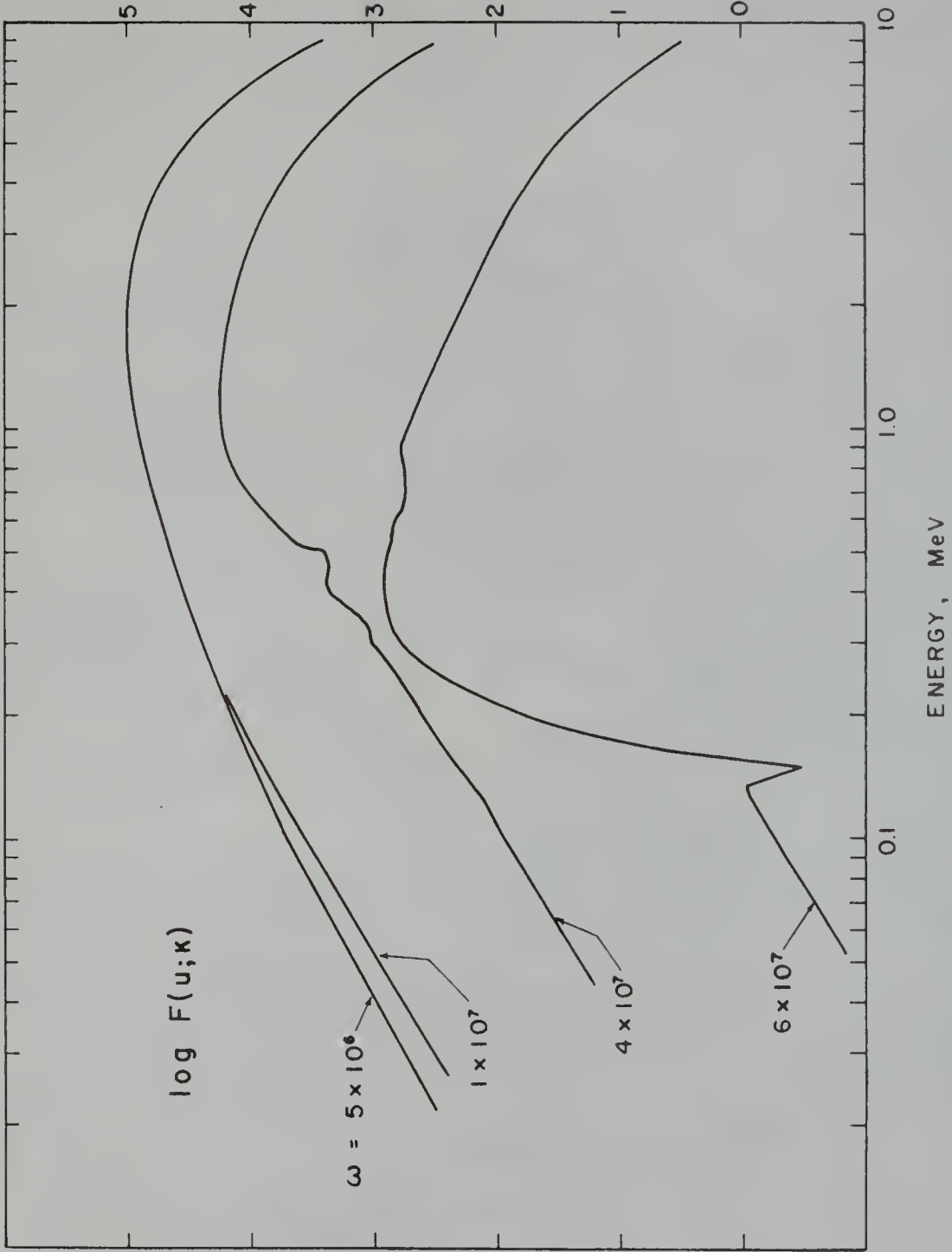


Figure 4.3 Eigenfunction energy spectra for moderate to high frequencies.

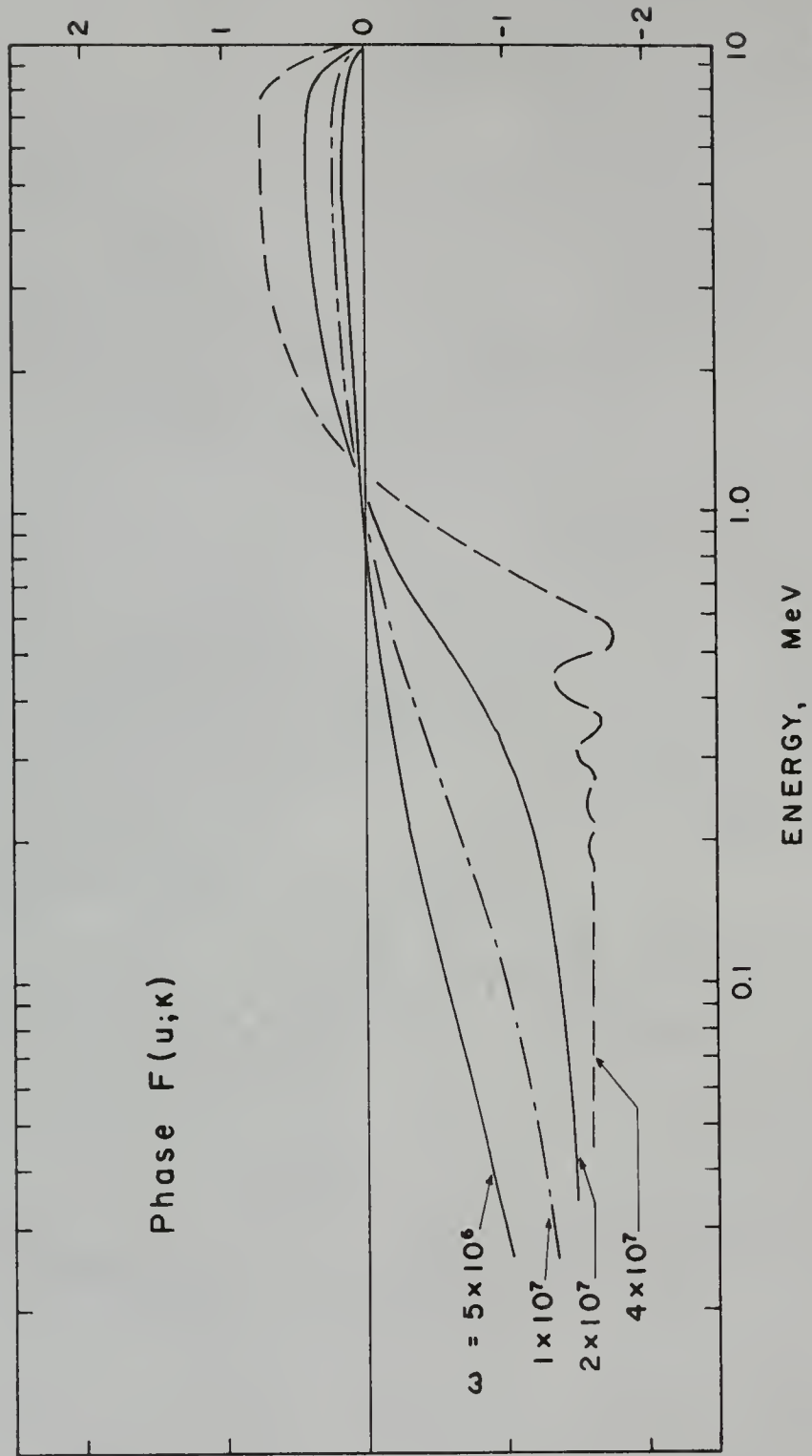


Figure 4.4 Eigenfunction phases for moderate frequencies (in radians).

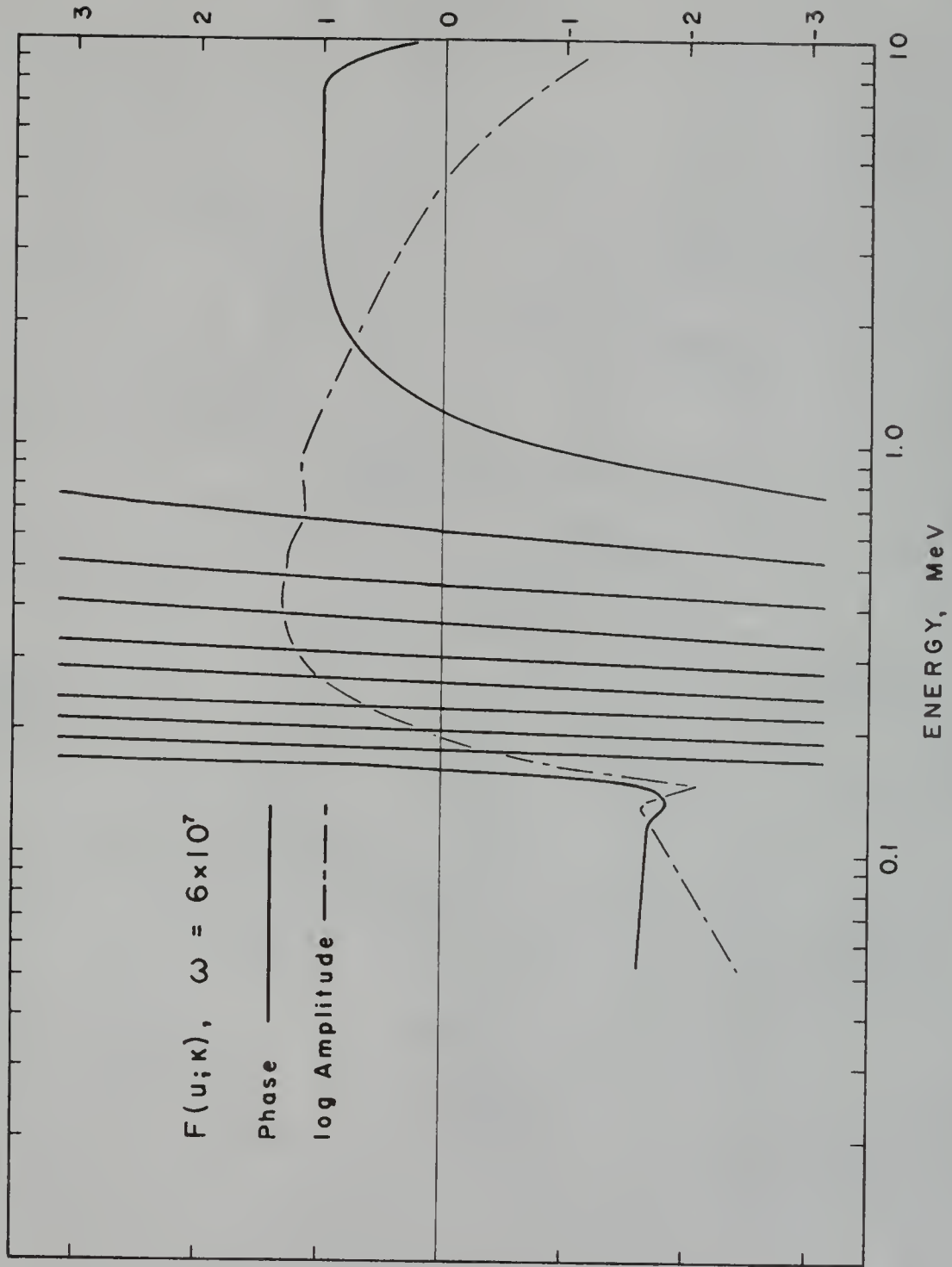


Figure 4.5 High frequency eigenfunction phase and amplitude relationship.

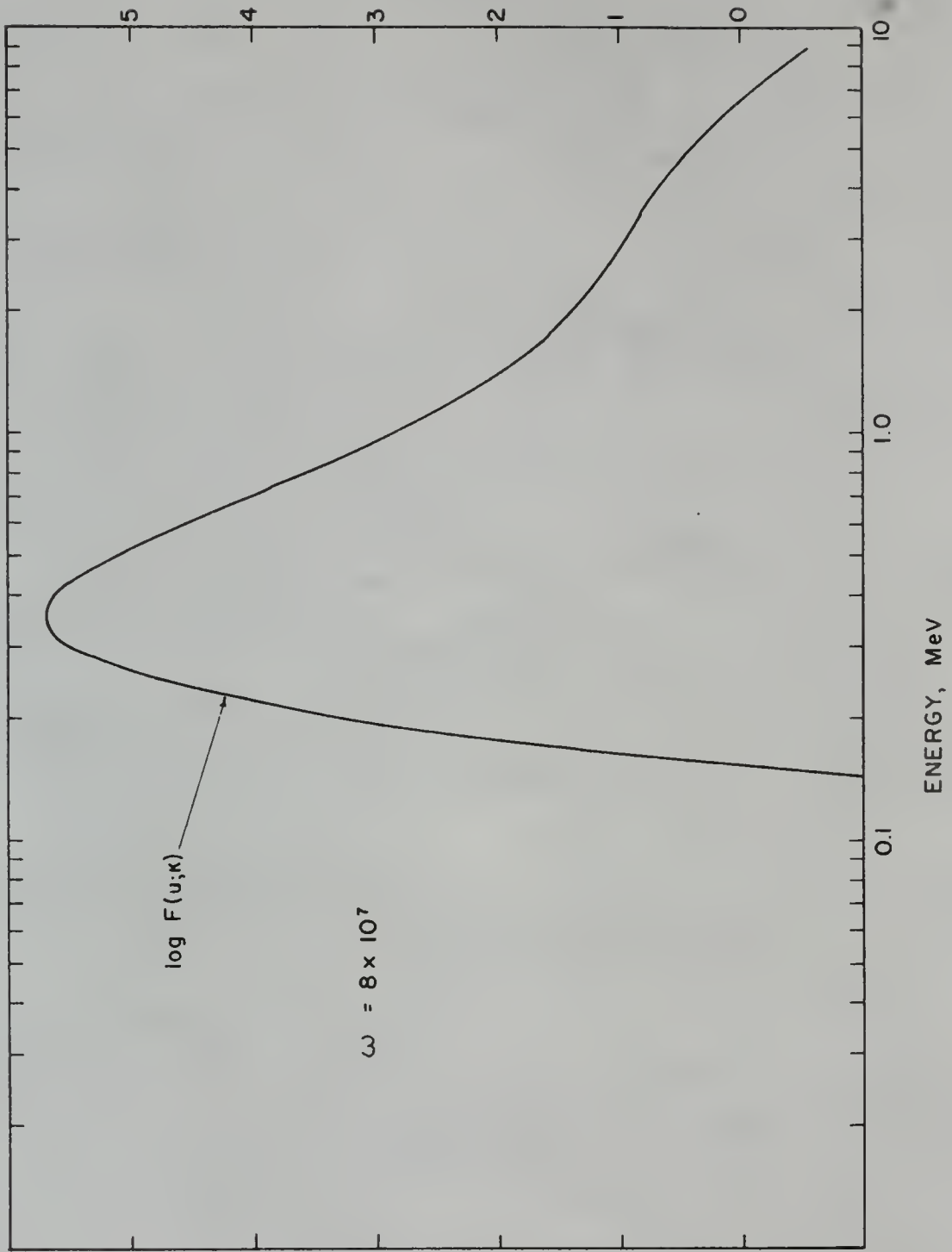


Figure 4.6 Eigenfunction energy spectrum for frequency approaching the critical frequency.

neutrons in energy occurs at an energy value corresponding to the maximum of $(a-\kappa)^{-1}$, so that we begin to see the onset of continuum-like behavior. The phase corresponding to Figure 4.6 is not plotted; the eigenfunction exhibits lagging of phase (which will result in rapid oscillations of phase relationships over small ranges of energy) even more severe than that shown in Figure 4.5, beginning at about 0.8 MeV and extending to lower energies.

Peaking of the eigenfunction at the energy which maximizes $(a-\kappa)^{-1}$ can be understood by noting the μ -dependent form of the eigenfunction, Eq. (4.2). Recalling that $(a-\mu\kappa)^{-1}$ has a pole for $\mu = 1$ at the edge of the continuum, it is apparent that the discrete eigenfunction will become more nearly monoenergetic and forward-directed as ω approaches the critical frequency, due to the presence of this factor (note that it is also a coefficient of each of the collision integrals in §).

Evidently, then, as ω approaches the critical frequency it will become increasingly difficult to excite a discrete mode without strongly exciting continuum modes as well, in view of the lack of phase coherence of the eigenfunction in its maximum amplitude region. Recalling previous remarks on the apparent interference of continuum eigenfunctions to produce almost-separable mode behavior, it is probable that the continuum contribution to the propagated wave will be important in this case as well. It would be interesting if a high-frequency wave were to assume asymptotically a sharp energy distribution as in Figure 4.6; this does not, however, seem likely. Further investigation of this question will require methods for determining superimposed contributions of both discrete and continuum modes.

CHAPTER V

SUMMARY AND CONCLUSIONS

Summary

This dissertation has explored the transport formulation of the fast neutron wave and pulse propagation problem in slab geometry. Both multiplying and nonmultiplying media were considered. The spectrum of the wave Boltzmann operator and formal expressions for discrete and continuum eigenfunctions were obtained. It was found that while the presence of the scattering operator prevents direct application to the fast case of the analytic techniques which have been used for the thermal regime, a consistent extension of the thermal eigenfunction results is found which takes scattering into consideration. In this extension an operator appears which arises from inversion of the identity minus the scattering operator; the inverse operator has a Neumann series expansion for eigenvalues in the discrete spectrum. This expansion represents familiar iterated collision intervals, each integral weighted by a transport factor $(a-\mu\kappa)^{-1}$. The same operator inverse appears in the continuum eigenfunction expressions; while the situation there regarding the existence of the Neumann series inverse is more tentative, apparently there is physical and some mathematical justification for interpreting the inverse operator in this way. All eigenfunction expressions reduce to forms consistent with more well-established thermal

results in the limit of vanishing scattering cross section. Qualitative correspondence was noted with the few transport studies dealing with the static transport equation in fast multiplying and nonmultiplying media.

A basis for application of the wave transport results to finite regions was established by generalizing the transfer matrix formalism to energy-dependent isotropic interaction models. The complete equivalence of the isotropic Boltzmann equation and transport transfer matrix eigenfunction problems was demonstrated, and specific simple relationships between the two sets of eigenfunctions were obtained. These results are more general than the scope of the present fast wave investigation; since the specific form of the interaction kernel does not enter into the expressions, they apply equally well to fast or thermal regimes.

Finally, dispersion law and discrete eigenfunction expressions were considered in detail for separable and degenerate fission kernel models, an efficient algorithm for fundamental mode computation was presented, and specific expressions were developed for an isotropic elastic scattering and inelastic scattering model. Eigenfunctions were shown to consist of a superposition of solutions to wave transport slowing-down equations, each having the fission spectrum for one fissionable species as a source. Eigenvalues were found from the dispersion law, which was seen to be in the form of a modal criticality condition. Illustrative calculations were performed for a one-term isotropic elastic scattering, separable fission kernel model. The discrete eigenfunctions were found to have an energy distribution very similar to the fission spectrum at low frequencies, with small phase variation over the total energy range. At frequencies approaching the critical frequency, the

eigenfunctions exhibited strong peaking in energy and in the forward direction, accompanied by rapid phase variation with energy in the vicinity of the peak.

Conclusions and Suggestions for Future Work

The theory of fast neutron wave and pulse propagation has received almost no attention, and the application of transport theory to the fast neutron regime has received little. While the difficulty of performing analysis in the fast regime is acknowledged, nevertheless this situation is both surprising and unfortunate. In this dissertation an attempt has been made to obtain specific results where possible, and to establish directions which future investigations should take.

Theoretically, the situation with respect to the discrete spectrum and eigenfunctions appears to be well in hand, at least for moderate frequencies. This is not to say that interesting work does not remain; as noted before, very little numerical work exists on wave and pulse propagation in fast multiplying media, and evidently there is no experimental data available. The qualitative effects of material composition, cross-section characteristics and other parameters upon fundamental mode propagation have yet to be explored. In particular it should be ascertained whether traditional propagation experiments are sensitive to parameters which may be of interest in fast reactor kinetics and safety analysis. The implications of the peaked energy and direction exhibited by the discrete eigenfunctions for very high frequencies should be developed. It is possible that this behavior is simply an indication that discrete modes are not excited strongly, relative to the continuum modes, as frequencies approach the critical frequency. On

the other hand if waves should be found to exhibit such behavior for deep penetration this would be an interesting result; this subject could be further explored theoretically, and studied experimentally by means of energy-sensitive detectors.

To investigate high frequency waves in multiplying media, propagation in finite regions, and, of course, propagation in nonmultiplying media it will be necessary to take into account the continuum eigenfunctions in implementing an eigenfunction expansion approach (or the equivalent transfer matrix formalism). Whether such an approach can succeed in practice is a question which must be addressed by further investigations. Either of two generic methods which suggest themselves may be employed in treating the continuum; one may attempt to extend analytic techniques, such as the generalized analytic function method, to the fast case, or one may search for some approximation to the continuum eigenfunctions which discretizes the continuum and which is amenable to numerical implementation. The former suggestion involves significant extrapolation of present mathematical techniques, and may well prove too complicated in realistic applications, though valuable for phenomenological understanding through treatment of modeled interactions. The latter suggestion has, to the best knowledge of this author, no precedent.

These comments are not intended as a criticism of the singular eigenfunction approach as applied in particular to the fast neutron regime, since the method is far from fully developed for thermal analysis. Indeed, it is not yet clear whether the singular eigenfunction method will prove useful as a framework for numerical application to practical problems [29,50] in the thermal regime although it is of

course valuable both as a source of exact solutions against which to check other methods and as a means of understanding transport effects.

It is apparent from the forms of the continuum eigenfunctions for both fast multiplying and nonmultiplying cases that it is necessary to understand the slowing-down continuum eigenfunctions in order to understand all continuum phenomena. These eigenfunctions are important not only as the appropriate ones for the important problem of propagation in passive media, but also since they evidently are associated with the modal excitation mechanism for the continuum for multiplying media. In this connection it should be remarked that the interpretation which was given for continuum modes can be viewed in rather general terms by recalling that the "Case's method" eigenfunction expression, e.g., Eq. (2.16), looks very much like an inhomogeneous Boltzmann equation with a delta-function source; interpretation of the singular eigenfunctions in terms of modal excitation by such a streaming source therefore may be illusory. On the other hand, in the absorption-only case it is obvious that this interpretation is correct. Whether this is an accurate or helpful approach to understanding the continuum is a matter which can be resolved only by detailed investigation, just as the formal eigenfunction expressions themselves remain to be substantiated, either theoretically or by application and comparison with other methods. Since slowing-down eigenfunctions appear in all continuum expressions, a logical starting point for investigation of continuum phenomena would be to explore the slowing-down problem for a simple elastic scattering or comparable kernel. Results of such a study would be not only of theoretical interest but also helpful in interpreting pulse propagation experiments in heavy scattering materials [11-13].

Mention should be made of the possibility of extending the present analysis to systems having finite transverse dimensions, and to other geometries. The essential analytic novelty presented here is the inversion of the scattering operator; applying this technique to other transport problems (again, see McCormick and Kuščer [29]) should be straightforward. Also it should be repeated that the methods presented here are applicable to thermalization problems in which separable or degenerate kernels are employed.

APPENDICES

APPENDIX A

Introduction

In Chapter III various transfer matrix operators in slab geometry are expressed in terms of WBE eigenfunctions, and the basic equivalence between the eigenfunction expansion and transfer matrix techniques is emphasized. Actually, the transfer matrix approach is a family of methods which may be applied to fairly arbitrary geometries and to physical quantities other than the neutron flux. In this appendix the transfer matrix will be derived from basic principles and its general properties will be discussed, essentially following Aronson and Yarmush [64] and Aronson [65]. It will be found necessary to introduce the geometry explicitly in order to progress beyond fundamental considerations. The most general expression for the basic wave-transport transfer matrix operators in slab geometry then will be obtained.

General Formalism

The transfer matrix approach to neutron propagation differs from the more common Boltzmann equation technique in that the latter is concerned with a pointwise description of the transport process within a medium, while the transfer matrix method considers the problem of transport through a medium in terms of incident and emergent fluxes at the boundaries. In this respect it greatly resembles the invariant imbedding technique, and in fact there is considerable common ground between the

two [71]. Initially we consider a region of space occupied by a homogeneous isotropic medium through which a neutron flux may propagate. (Here the flux will be the usual energy and direction-dependent "angular flux" in either time-dependent or Fourier-transformed representation. Obviously, more restricted models also may be treated.) All that is required at this point is that one be able to assign two "sides" to the region. These sides will be arbitrarily referred to as "left" and "right." No problem arises with the formalism in the treatment of voids and reentrant configurations, provided that all relevant surfaces of the region under consideration are assigned to either the left or right sides. In some cases, as, for example, for finite bodies, designation of the two "sides" may be entirely arbitrary, but for such bodies, once boundaries are assigned the transfer matrix is defined unambiguously. Since only slab geometry will be considered in detail here, this aspect of the method will not be pursued; it will be assumed that appropriate sides may be designated for all regions of interest [78].

The transfer matrix may be defined as the linear operator which relates entering and emerging fluxes at one side of a region to the corresponding fluxes at the other side. This situation is represented schematically in Figure A.1. Here, for example, $\phi_+(L) \equiv \phi_+(\vec{r}_L, E, \vec{\Omega}, t)$, where \vec{r}_L is the coordinate of a point on the left surface of the region; motion in the positive sense is taken to be from left to right. Thus $\phi_+(L)$ and $\phi_-(R)$ are entering fluxes, while $\phi_-(L)$ and $\phi_+(R)$ are emerging. Entering and emerging may, of course, be defined unambiguously by

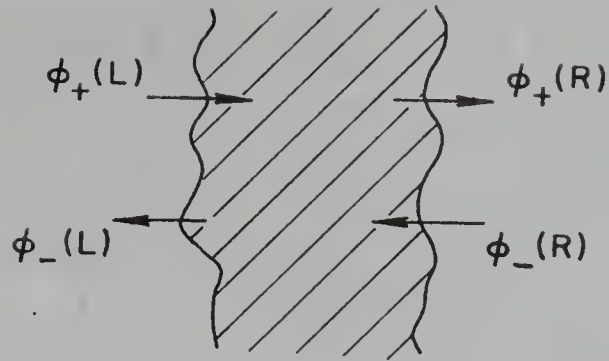


Figure A.1 Entering and emerging fluxes for a single region.

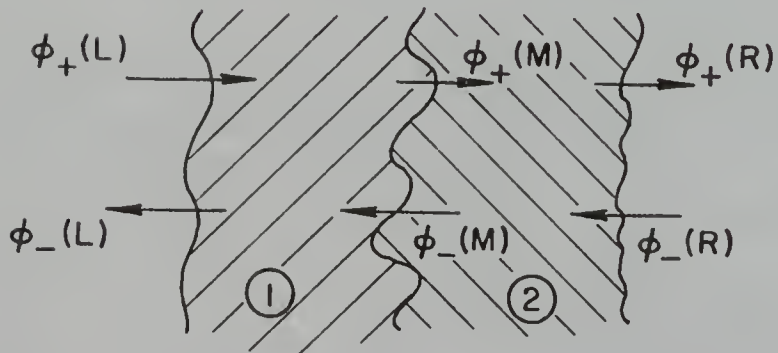


Figure A.2 Entering and emerging fluxes for adjacent regions.

$$\vec{\Omega} \ni \vec{\Omega} \cdot \vec{n}_s > 0 \quad \Rightarrow \text{emerging}$$

$$\vec{\Omega} \ni \vec{\Omega} \cdot \vec{n}_s < 0 \quad \Rightarrow \text{entering}$$

where \vec{n}_s is the outward-directed unit vector normal to the surface at any point.

The transfer matrix equation* for Figure A.1 may be written

$$\begin{bmatrix} \phi_+(R) \\ \phi_-(R) \end{bmatrix} = H_{L \rightarrow R} \begin{bmatrix} \phi_+(L) \\ \phi_-(L) \end{bmatrix} \quad (\text{A.1})$$

or more compactly,

$$\phi(R) = H_{L \rightarrow R} \phi(L) \quad (\text{A.2})$$

where the transfer matrix H is a 2×2 matrix of linear operators when the fluxes are resolved into entering and emerging fluxes, as in Eq. (A.1). Linearity of H requires that no flux-independent sources be imbedded within the region, although fission sources, which are linear functions of the flux, may be taken into account in H. This linearity condition has further implications with regard to the nature of the region described. Since nonfission sources must be exterior to the

*In this appendix symbols for matrix and operator quantities will be written without a tilde, since there is no possibility of confusion between an operator and its elements.

region, it is necessary that the region be well defined by its bounding surfaces. These topological nuances will not be of interest here; it is sufficient to note that Eq. (A.1) certainly will be applicable to a singly-connected region totally bounded by its "right" and "left" sides.

Algebra of the H-Matrix

Consider two adjacent regions, 1 and 2, completely bounded by "left" and "middle," and "middle" and "right" sides, respectively. This situation is diagrammed in Figure A.2. Applying Eq. (A.1) to regions 1 and 2 we may write

$$\begin{aligned}\phi(M) &= H_1\phi(L) \\ \phi(R) &= H_2\phi(M) \quad .\end{aligned}\tag{A.3}$$

Combining these two equations,

$$\phi(R) = H_2H_1\phi(L) \quad .\tag{A.4}$$

Evidently the transfer matrix for the combined regions 1 and 2, H_{12} , is given by the matrix operator equation

$$H_{12} = H_2H_1\tag{A.5}$$

and similarly

$$H_n \text{ regions} = H_n H_{n-1} \cdot \cdot \cdot H_2 H_1. \quad (\text{A.6})$$

Obviously transfer matrices do not in general commute. Furthermore, it is apparent that for any region, in the limit of vanishing width the transfer matrix must tend to the identity operator:

$$\lim_{\text{"width"} \rightarrow 0} H = I. \quad (\text{A.7})$$

These characteristic properties must be satisfied by all transfer matrices [64].

Form of the H-Matrix: T and R Operators

We will now express the transfer matrix in terms of linear operators which relate emerging fluxes to incident fluxes. This may be done without any further restrictions on the type of region considered. Figures A.3 and A.4 illustrate the situations relevant to the ideas of transmission and reflection, respectively. An incident flux $\phi_+(L)$ will give rise to an emergent flux $\phi_+(R)$ which may be regarded as transmitted, and $\phi_-(L)$ which may be regarded as reflected. In other words, any entrant flux at one side will produce an emergent flux distribution over the entire surface; the flux emerging from the same side is termed "reflected," and flux emerging through the other side is "transmitted." These distinctions apply even though the surface configuration may be such that the terms are not particularly descriptive of the physical

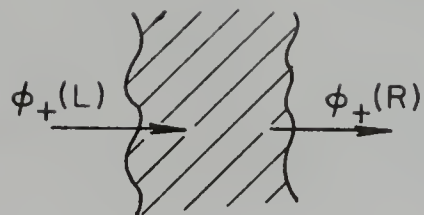


Figure A.3 Transmission.

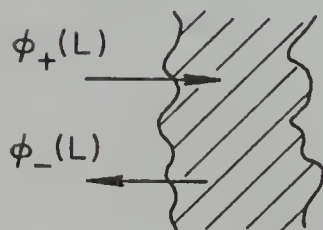


Figure A.4 Reflection.

processes. Transmission and reflection operators may be defined for $\phi_+(L)$ incident, as in Figures A.3 and A.4, by the relations

$$\phi_+(R) = T\phi_+(L) \quad (\text{A.8})$$

$$\phi_-(L) = R\phi_+(L) \quad (\text{A.9})$$

where T and R may be used to treat both attenuating and multiplying media. These operators are in fact Green's functions for the energy and direction-dependent flux, expressing outward-directed fluxes at surface points of the region in terms of the "source" $\phi_+(L)$, which is completely arbitrary. That is,

$$T \equiv T(\vec{r}_L, \vec{\Omega}_L, E_L \rightarrow \vec{r}'_R, \vec{\Omega}'_R, E'_R; t' - t) \quad (\text{A.10})$$

and

$$R \equiv R(\vec{r}_L, \vec{\Omega}_L, E_L \rightarrow \vec{r}'_L, \vec{\Omega}'_L, E'_L; t' - t). \quad (\text{2.11})$$

A corresponding pair of operators may be defined for an incident flux distribution at the right, $\phi_-(R)$:

$$\phi_-(L) = T^*\phi_-(R) \quad (\text{A.12})$$

$$\phi_+(R) = R^*\phi_-(R) \quad (\text{A.13})$$

where the asterisks represent transmission and reflection in the sense of right-to-left. These operators in general will differ from their

unstarred counterparts. Equations (A.8), (A.9), (A.12), and (A.13) may be combined to give the emergent fluxes for arbitrary incident flux distributions over both faces:

$$\phi_+(R) = T\phi_+(L) + R^*\phi_-(R) \quad (\text{A.14})$$

$$\phi_-(L) = R\phi_+(L) + T^*\phi_-(R). \quad (\text{A.15})$$

But Eqs. (A.12) and (A.13) may be solved formally for the fluxes at the right face in terms of those at the left. (In the following it will be assumed that all required inverse exist; in applications, existence may impose restrictions on the problem. For example, subcriticality may be required.)

$$\phi_-(R) = -T^{*-1}R\phi_+(L) + T^{*-1}\phi_-(L) \quad (\text{A.16})$$

$$\phi_+(R) = (T-R^*T^{*-1}R)\phi_+(L) + R^*T^{*-1}\phi_-(L) \quad (\text{A.17})$$

preserving the correct sequence in all operator manipulations.

If the fluxes are now written in vector form and the operators combined into a matrix, we have

$$\begin{bmatrix} \phi_+(R) \\ \phi_-(R) \end{bmatrix} = \begin{bmatrix} T-R^*T^{*-1}R & R^*T^{*-1} \\ -T^{*-1}R & T^{*-1} \end{bmatrix} \begin{bmatrix} \phi_+(L) \\ \phi_-(L) \end{bmatrix} \quad (\text{A.18})$$

which is precisely the transfer matrix equation, with the identification

$$H = \begin{bmatrix} T - R^*T^{*-1}R & R^*T^{*-1} \\ -T^{*-1}R & T^{*-1} \end{bmatrix}. \quad (\text{A.19})$$

This is the most general form of the transfer matrix in terms of the four transmission and reflection operators [64].

Two-Region Transfer Matrix

Equation (A.5) now may be applied to the transfer matrices for two adjacent regions, H_1 and H_2 , as in Figure A.2. The transfer matrix of the combined region, H_{12} , is the matrix product of two matrices such as in Eq. (A.19); the elements of the product matrix bear the same relationship to the combined region as the corresponding elements in Eq. (A.19) bear to a single region. For example, we may compute the lower right-hand element

$$\begin{aligned} T_{12}^{*-1} &= -T_2^{*-1} R_2 R_1^* T_1^{*-1} + T_2^{*-1} T_1^{*-1} \\ &= T_2^{*-1} \left(I - R_2 R_1^* \right) T_1^{*-1}. \end{aligned} \quad (\text{A.20})$$

Inverting this expression,

$$T_{12}^* = T_1^* \left(I - R_2 R_1^* \right)^{-1} T_2^*, \quad (\text{A.21})$$

which gives the operator for transmission through both slabs from right to left, provided that the required inverse exists. Then, if $(I - R_2 R_1^*)^{-1}$ may be expanded in a Neumann series, we have

$$T_{12}^* = T_1^* \sum_{n=0}^{\infty} \left(R_2 R_1^* \right)^n T_2^* . \quad (\text{A.22})$$

Physically, Eq. (A.22) may be interpreted as in Figure A.5. The total transmitted flux is the sum of contributions from flux which has suffered n pairs of internal reflections before exiting through the left face. This is a well-known result which has been obtained previously by "particle-counting" arguments analogous to the one illustrated here.

Internal Sources

Sources external to the region of interest are expressed in terms of the entering fluxes which they generate at the surfaces of the region, and therefore enter implicitly into the formalism through $\phi_+(L)$ and $\phi_-(R)$. Fission sources are linear functions of the flux and therefore may be included directly in the transmission and reflection operators. Thus the only type of source which would occur as an inhomogeneous contribution to the transfer matrix equation would be a flux-independent source imbedded in the region. Such internal sources may be taken into account by expressing the sources in terms of the emerging fluxes which they generate at the left and right faces, Q_- and Q_+ , respectively, as

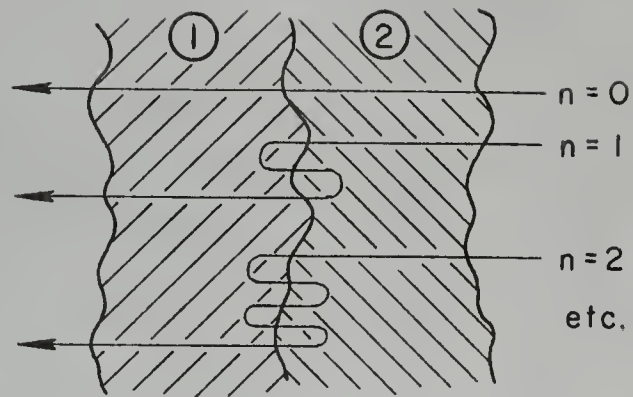


Figure A.5 Transmission through adjacent regions.

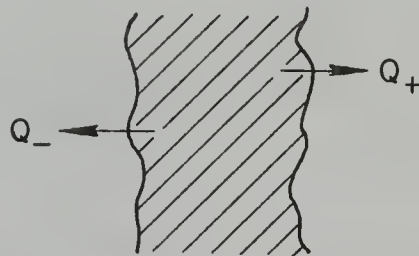


Figure A.6 Internal inhomogeneous sources.

in Figure A.6. Equations (A.14) and (A.15) may be modified to include the contributions of internal sources to the emerging fluxes:

$$\phi_+(R) = T\phi_+(L) + R^*\phi_-(R) + Q_+ \quad (\text{A.23})$$

$$\phi_-(R) = R\phi_+(L) + T^*\phi_-(R) + Q_- \quad (\text{A.24})$$

These two equations may be combined to give equations in $\phi_+(R)$ and $\phi_-(R)$ corresponding to Eqs. (A.16) and (A.17), but containing the source fluxes Q_+ and Q_- ; the resulting equations similarly may be arranged into matrix form as

$$\phi(R) = H\phi(L) + Q \quad (\text{A.25})$$

where the inhomogeneous source vector Q is found to be

$$Q = \begin{bmatrix} Q_+ & -R^*T^{*-1}Q_- \\ & -R^{*-1}Q_- \end{bmatrix} \quad (\text{A.26})$$

Transfer Matrix for Homogeneous Slabs

The rest of this development will apply specifically to homogeneous slabs of finite thickness in the x direction, and infinitely extensive in the y and z directions. (The condition of homogeneity is not as restrictive as it may seem, since slabs which vary in composition in the

x direction may be approximated arbitrarily well by layers of homogeneous sub-slabs.) It is assumed that all incident fluxes and all source distributions are

- (a) constant with respect to y and z
- (b) constant with respect to azimuthal angle about x.

In this case the angular neutron flux becomes a function only of x, E, μ , and t, where μ is the usual cosine of angle with respect to the x axis. Values of μ will be taken to range from 0 to 1 for both ϕ_+ and ϕ_- . This designation is convenient as well as unambiguous, since the information regarding the "direction" of the fluxes, normally contained in the sign of μ , is transferred to the subscripts + and -.

For a homogeneous slab with these symmetries imposed

$$T \equiv T(\mu_L, E_L \rightarrow \mu'_R, E'_R; \tau; t'-t) = T^*(\mu_R, E_R \rightarrow \mu'_L, E'_L; \tau; t'-t) \quad (\text{A.27})$$

and

$$R \equiv R(\mu_L, E_L \rightarrow \mu'_L, E'_L; \tau; t'-t) = R^*(\mu_R, E_R \rightarrow \mu'_R, E'_R; \tau; t'-t) \quad (\text{A.28})$$

where τ is a slab width. Since ϕ_+ and ϕ_- do not depend upon position on the surface, T, R, and H have spatial dependence only through slab width, as expressed in the above equations. Equality of the forward and backward operators is the result both of the symmetry of the physical situation and of the stipulation $\mu \in (0,1]$. An immediate consequence of this is that

$$H = H^* \quad (\text{A.29})$$

and hence for two adjacent slabs, 1 and 2, of identical composition

$$H_{12} = H_{12}^* = (H_2 H_1)^* = H_1^* H_2^* = H_1 H_2 \quad (\text{A.30})$$

so that in this case

$$H_{12} = H_1 H_2 = H_2 H_1 = H_{21}. \quad (\text{A.31})$$

This equality also is obvious on physical grounds, since the composite slabs (1 + 2) and (2 + 1), and the total slab (12), all are indistinguishable with respect to neutron transport properties.

The commutation property of Eq. (A.31) is useful in determining the functional dependence of H upon slab width for homogeneous slabs, when width is regarded as a variable parameter. For slab width $x + \Delta x$,

$$H(x + \Delta x) = H(x)H(\Delta x) \quad (\text{A.32})$$

independent of the manner in which Δx , which we now may regard as an arbitrary increment, is selected. The variation of H with respect to slab width then may be written

$$H(x + \Delta x) - H(x) = H(x) [H(\Delta x) - I] \quad (\text{A.33})$$

so

$$\frac{H(x + \Delta x) - H(x)}{\Delta x} = H(x) \left[\frac{H(\Delta x) - I}{\Delta x} \right]. \quad (\text{A.34})$$

We now follow the usual procedure of passing to the limit $\Delta x \rightarrow 0$.

Define

$$W \equiv \lim_{\Delta x \rightarrow 0} \frac{I - H(\Delta x)}{\Delta x}. \quad (\text{A.35})$$

That W exists is at least plausible, since the transfer matrix is required by Eq. (A.7) to have the property

$$\lim_{\Delta x \rightarrow 0} H(\Delta x) = I. \quad (\text{A.36})$$

An explicit form for W will be obtained by use of Eq. (A.35).

In the limit $\Delta x = 0$, Eqs. (A.34) and (A.35) give

$$\frac{\partial H(x)}{\partial x} = -WH \quad (\text{A.37})$$

(note that W and H commute) which, with the initial condition $H(0) = I$ yields the form

$$H(x) = e^{-xW} \quad (\text{A.38})$$

for a homogeneous slab of width x . W is an operator, whereas slab width now appears only as a scalar multiplier. We now have two expressions for H . Equation (A.19) becomes

$$H = \begin{bmatrix} T - RT^{-1}R & RT^{-1} \\ -T^{-1}R & R^{-1} \end{bmatrix} \quad (\text{A.39})$$

taking into account the symmetry of the homogeneous slab geometry (Eqs. (A.27) and (A.28)). Equations (A.38) and (A.39) may be exploited to determine an explicit expression for W . Now the transmission and reflection operators must have a Taylor series development in terms of slab width x ; in the limit $x \rightarrow 0$ we should have to first order in x

$$T = I - x\alpha + \dots, \quad (\text{A.40})$$

$$R = x\beta + \dots, \quad (\text{A.41})$$

since T should tend to the identity operator and R should tend to the null operator as the slab width becomes vanishingly small. Once again, α and β are operators (which we must deduce from other considerations), while x is a scalar. When these expressions are inserted into Eq. (A.39), the corresponding equation for H becomes, to first order in x ,

$$\lim_{x \rightarrow 0} H = \begin{bmatrix} I - x\alpha & x\beta \\ -x\beta & I + x\alpha \end{bmatrix}. \quad (\text{A.42})$$

Then from Eq. (A.35)

$$W = \begin{bmatrix} \alpha & -\beta \\ \beta & -\alpha \end{bmatrix} . \quad (\text{A.43})$$

It should be noted that W is dependent of slab width, since the operators α and β depend only on the properties of the slab medium. Thus through the introduction of slab geometry it is possible to reduce the transfer matrix from a form containing rather formidable Green's functions in all space and velocity variables to one in which the spatial coordinate enters only through slab thickness, and only as a scalar parameter.

The Operators α and β

The transfer matrix equation for a homogeneous slab extending from 0 to x may be written compactly

$$\phi(x) = H(x)\phi(0) . \quad (\text{A.44})$$

Differentiating and making use of Eq. (A.37),

$$\frac{\partial \phi(x)}{\partial x} = \frac{\partial H(x)}{\partial x} \phi(0) = -WH(x)\phi(0) \quad (\text{A.45})$$

so that by use of Eq. (A.44)

$$\frac{\partial \phi(x)}{\partial x} = -W\phi(x) . \quad (\text{A.46})$$

This equation is especially interesting since it is a differential operator equation for the flux vector at the right surface only. While Eq. (A.46) was obtained for a slab of width x , it applies equally well to the flux at a surface located at coordinate x , embedded within a slab of arbitrary width τ , as in Figure A.7. Thus Eq. (A.46) is essentially a pair of coupled differential operator equations for the forward and backward-directed angular fluxes, $\phi_+(x)$ and $\phi_-(x)$, at x within the slab. For example, the equation for the ϕ_+ component is

$$\frac{\partial \phi_+(x)}{\partial x} = -\alpha \phi_+(x) + \beta \phi_-(x) \quad (\text{A.47})$$

It is obvious that the operators α and β must contain the physics of neutron interactions in the slab, and hence contain cross section, scattering, and multiplication operators. The fact that Eq. (A.47) is a partial differential equation at a single interior coordinate x enables us to determine the form of α and β from the equivalent differential or differentio-integral representation of the problem.

Once α and β have been determined, Eqs. (A.38) and (A.43) give the operator matrices W and H , and in principle these could be applied to computations without further development. However, the operator W appears exponentially in H , so that the utility of this direct approach

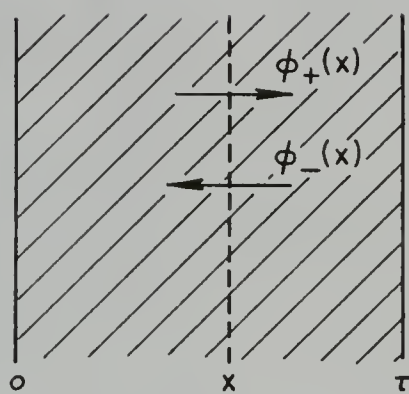


Figure A.7 Fluxes at an internal coordinate surface.

depends on rapid convergence of terms of the series $(\tau W)^n$. While this may be practical for some problems in which the full transfer matrix is required, especially for thin slabs, an alternative approach is to diagonalize W .

Diagonalization of the Transfer Matrix

Suppose a basis has been found upon which W is diagonal; that is, for some matrix S ,

$$S^{-1}WS = A \quad (\text{A.48})$$

where A is the diagonal operator consisting of the spectrum of W . Then

$$W = SAS^{-1} \quad (\text{A.49})$$

and

$$H = e^{-\tau W} = e^{-\tau SAS^{-1}} \quad (\text{A.50})$$

so that

$$H = Se^{-\tau A}S^{-1} \quad (\text{A.51})$$

That is, if the spectrum and the eigenfunctions of W can be determined (the eigenfunctions constitute the matrix S), the exponential behavior of H with respect to τ will enter only through $e^{-\tau A}$, which is itself diagonal.

Rather than attempting to solve an eigenvalue equation for a 2×2 matrix of operators, it is more convenient to consider first an auxiliary eigenvalue problem. Define

$$\sigma \equiv \alpha + \beta \quad (\text{A.52})$$

$$\delta \equiv \alpha - \beta \quad (\text{A.53})$$

and their product operator, $\sigma\delta$. Suppose that this operator may be diagonalized,

$$\Gamma^2 = X^{-1} \sigma\delta X, \quad (\text{A.54})$$

where Γ^2 is the diagonal operator consisting of eigenvalues of $\sigma\delta$. Then it may be verified by substitution that, formally at least, the following equations result:

$$A = \begin{bmatrix} \Gamma & 0 \\ 0 & -\Gamma \end{bmatrix} \quad (\text{A.55})$$

$$S = \frac{1}{2} \begin{bmatrix} B_+ & B_- \\ B_- & B_+ \end{bmatrix} \quad (\text{A.56})$$

$$S^{-1} = \frac{1}{2} \begin{bmatrix} C_+ & C_- \\ C_- & C_+ \end{bmatrix} \quad (\text{A.57})$$

where

$$B_{\pm} = X \pm \xi \quad (\text{A.58})$$

$$C_{\pm} = X^{-1} \pm \xi^{-1} \quad (\text{A.59})$$

and

$$\xi \equiv \delta X \Gamma^{-1} = \sigma^{-1} X \Gamma. \quad (\text{A.60})$$

Explicitly,

$$W = SAS^{-1} = \frac{1}{4} \begin{bmatrix} B_+ & B_- \\ B_- & B_+ \end{bmatrix} \cdot \begin{bmatrix} \Gamma & 0 \\ 0 & -\Gamma \end{bmatrix} \cdot \begin{bmatrix} C_+ & C_- \\ C_- & C_+ \end{bmatrix} \quad (\text{A.61})$$

and

$$H = Se^{-\tau A} S^{-1} = \frac{1}{4} \begin{bmatrix} B_+ & B_- \\ B_- & B_+ \end{bmatrix} \cdot \begin{bmatrix} e^{-\tau \Gamma} & 0 \\ 0 & e^{\tau \Gamma} \end{bmatrix} \cdot \begin{bmatrix} C_+ & C_- \\ C_- & C_+ \end{bmatrix}. \quad (\text{A.62})$$

These are the diagonalization operator equations which are discussed in detail in Chapter III.

Transmission and Reflection Operators

In most applications it will be necessary to compute transmission and reflection operators as well as (or in place of) the full transfer matrix H . In fact, the most utilitarian feature of the formalism, aside from its generality, may be that it provides relationships between transmission and reflection operators and eigenfunctions of the more familiar

neutron transport equations. Expressions for these operators in terms of the diagonalization operators may be deduced by comparing the form of H as a function of T and R , Eq. (A.39), with Eq. (A.62). With a little manipulation one obtains

$$T(\tau) = 4C_+^{-1} e^{-\tau\Gamma} E_+^{-1}(\tau) \quad (\text{A.63})$$

and

$$R(\tau) = E_-(\tau) E_+^{-1}(\tau) \quad (\text{A.64})$$

defining

$$E_{\pm}(\tau) \equiv B_{\pm} + B_{\mp} e^{-\tau\Gamma} U e^{-\tau\Gamma} \quad (\text{A.65})$$

and

$$U \equiv C_- C_+^{-1} = - B_+^{-1} B_- \quad (\text{A.66})$$

which permit computation of T and R from operators related to the physical properties of the slab medium through $\sigma\delta$ and the basic operators α and β .

Wave Transport Form of α and β

To obtain α and β in a wave transport representation, we return to Eq. (A.47). Writing α and β as integral operators (recalling that T and R and thus, from Eq. (A.40), α and β are defined over $\mu \in (0,1]$) with kernels K_{α} and K_{β} , Eq. (A.47) becomes

$$\begin{aligned}
\frac{\partial \phi_+(x, \mu, E, \omega)}{\partial x} &= - \int_0^\infty dE' \int_0^1 d\mu' K_\alpha(E', \mu' \rightarrow E, \mu; \omega) \phi_+(x, \mu', E', \omega) \\
&\quad + \int_0^\infty dE' \int_0^1 d\mu'' K_\beta(E', \mu'' \rightarrow E, \mu; \omega) \phi_-(x, \mu'', E', \omega).
\end{aligned}
\tag{A.67}$$

Now in similar notation the WBE is

$$\left[\mu \frac{\partial}{\partial x} + a(E, \omega) \right] \phi(x, \mu, E, \omega) = \int_0^\infty dE' \int_{-1}^1 d\mu' K_{BE}(E', \mu' \rightarrow E, \mu) \phi(x, \mu', E', \omega)
\tag{A.68}$$

including all interaction terms in the kernel K_{BE} . Rearranging,

$$\frac{\partial \phi}{\partial x} = - \frac{a}{\mu} \phi + \frac{1}{\mu} \int_0^\infty dE' \int_{-1}^1 d\mu' K_{BE}(E', \mu' \rightarrow E, \mu) \phi(x, \mu', E', \omega).
\tag{A.69}$$

When μ is restricted to the interval $(0, 1]$, $\phi(\mu) \equiv \phi_+(\mu)$. Furthermore, we have defined $\phi_-(\mu) \equiv \phi(-\mu)$. If the integral in Eq. (A.69) is divided into separate integrals over positive and negative μ' , and if the substitution $\mu'' = -\mu'$ is made in the negative integral,

$$\begin{aligned}
\frac{\partial \phi_+(x, \mu, E, \omega)}{\partial x} &= - \frac{a}{\mu} \phi_+ + \frac{1}{\mu} \int_0^\infty dE' \int_0^1 d\mu' K_{BE}(E', \mu' \rightarrow E, \mu) \phi_+(x, \mu', E', \omega) \\
&\quad + \frac{1}{\mu} \int_0^\infty dE' \int_0^1 d\mu'' K_{BE}(E', -\mu'' \rightarrow E, \mu) \phi_-(x, \mu'', E', \omega)
\end{aligned}
\tag{A.70}$$

where $\mu, \mu', \mu'' \in (0,1]$. Comparing Eqs. (A.67) and (A.70), we find that

$$\alpha \equiv \int_0^{\infty} dE' \int_0^1 d\mu' \left[\frac{a(E', \omega)}{\mu'} \delta(E' - E) \delta(\mu' - \mu) - \frac{1}{\mu} K_{BE}(E', \mu' \rightarrow E, \mu) \right] \quad (\text{A.71})$$

and

$$\beta \equiv \int_0^{\infty} dE' \int_0^1 d\mu' \left[\frac{1}{\mu} K_{BE}(E', -\mu' \rightarrow E, \mu) \right]. \quad (\text{A.72})$$

A similar treatment of the equation for $\phi_-(x)$ gives identical results. The kernel K_{BE} may, of course, contain any useful interaction model. This extends Aronson's work [64-70] to the most general wave transport representation of the one-dimensional slab transfer matrix.

APPENDIX B

Singularity of Inelastic Scattering Kernel Models

In this appendix an inelastic scattering kernel model [79,80] will be discussed which gives rise to an additional spectral contribution in the adjoint problem. This observation is due to Nikolaenko [14], who made use of the kernel in treating fast static transport problems.

We recall that in general the total isotropic scattering cross section is defined by

$$\Sigma_s(E) = \int_0^{\infty} \Sigma_s(E \rightarrow E') dE' . \quad (B.1)$$

For downscattering (either elastic or inelastic) this becomes

$$\Sigma_s(E) = \int_0^E \Sigma_s(E \rightarrow E') dE' . \quad (B.2)$$

We may write the kernel in question as

$$\begin{aligned} K_{in}(E \rightarrow E') &= g(E) h(E') & E > E' \\ &= 0 & E < E' \end{aligned} \quad (B.3)$$

For constant total inelastic scattering cross section, which Nikolaenko stipulates, we may write

$$\Sigma_{si}(E) = \text{const.} = \Sigma_{si} \int_0^E g(E') H(E') dE' \quad (\text{B.4})$$

so that the constant cross-section condition requires that

$$\int_0^E g(E') h(E') dE' = 1$$

or

$$\int_0^E h(E') dE' = \frac{1}{g(E)}. \quad (\text{B.5})$$

If $h(E)$ is bounded as $E \rightarrow 0$, $g(E)^{-1} \rightarrow 0$ in this limit. Thus while the forward inelastic scattering operator

$$\int_E^\infty dE' \Sigma_{si}(E' \rightarrow E) \cdot = \Sigma_{si} h(E) \int_E^\infty dE' g(E') \cdot \quad (\text{B.6})$$

has a bounded kernel for $E > 0$, the adjoint inelastic scattering operator

$$\int_0^E dE' \Sigma_{si}(E \rightarrow E') \cdot = \Sigma_{si} g(E) \int_0^E dE' h(E') \cdot \quad (\text{B.7})$$

clearly does not, as $g(E)$ is singular. Thus our inversion of the identity plus scattering operator fails for the adjoint WBE employing this model. In fact operator (B.7) has eigenfunctions [14] $g(E)^{1-\lambda}$ with corresponding eigenvalues $\frac{1}{\lambda}$ for all λ with $\text{Re}\lambda \geq 1$; hence the spectra of forward and adjoint Boltzmann operators evidently are different, and the entire approach based on construction of biorthogonal eigenfunction sets is unsuccessful in this case.

The question therefore becomes, is this unfortunate property a characteristic of inelastic scattering in general, or is it an artifact introduced by the specific model, Eq. (B.3)? Fortunately, the latter is true. From Eqs. (B.4) and (B.5) it is evident that the stipulation of constant total cross section at $E \rightarrow 0$, together with the form of the kernel (B.3), forces $g(E)$ to be singular. That is, it forces a divergent differential cross section, a result which is both inconvenient, as we have seen, and physically incorrect, since inelastic scattering does not occur at all for sufficiently low energies. (Nicolaenko avoids the difficulty of nonphysical results due to this divergence, as he does not apply the kernel below the inelastic scattering threshold; nevertheless the singularity does emerge, as we have seen, in the adjoint problem.) As we are dealing with fast systems we are in fact indifferent as to the precise form the inelastic scattering cross-section model at thermal energies and below, but we certainly are at liberty to allow the inelastic scattering cross section $\Sigma_{si}(E)$ to vanish as E^λ , for example, in some neighborhood of $E = 0$. This additional degree of freedom entirely resolves the present difficulty; retaining the kernel (B.3), we see that

$$g(E) = \frac{\Sigma_{si}(E)}{\int_0^E h(E') dE'} \quad (B.8)$$

so that for $E \rightarrow 0$ all that is required is that $\Sigma_{si}(E)$ vanish sufficiently rapidly.

It is apparent that the singularity of the kernel adjoint to (B.3) is not a property which generalizes to more accurate models of inelastic

scattering, and therefore the behavior of scattering kernels at the zero-energy limit should not necessarily hinder the development of transport theory for fast systems.

APPENDIX C

MACROSCOPICALLY ELASTIC SCATTERING: THE ELASTIC CONTINUUM

It has been shown in Chapter II that for "well-behaved" slowing-down operators the point spectrum of the wave Boltzmann operator is empty and that $\kappa \notin C$ belongs to the resolvent set. Here we discuss two limiting processes for scattering models which express concretely some of the ideas presented in connection with almost-separable mode behavior, and which give rise to continuous spectra for $\kappa \notin C$.

Duderstadt [32,33] discusses the effect of introducing the macroscopically elastic scattering operator of Eq. (2.25) upon the spectrum of the wave Boltzmann operator. Such a scattering operator arises in the theory of thermal neutron Bragg scattering in polycrystalline materials. In Chapter II its use in modeling elastic scattering from heavy nuclides was discussed briefly.

To pursue the ideas presented there, consider for simplicity an isotropic scattering kernel for the slowing-down WBE having macroscopically elastic and nonelastic terms

$$\Sigma_s(E' \rightarrow E) = \Sigma_{se}(E') \sigma(E', E, \Delta E) + \Sigma_{sne}(E' \rightarrow E) \quad (C.1)$$

where

$$\begin{aligned} \sigma(E', E, \Delta E) &= \frac{1}{\Delta E}, & E' - \Delta E \leq E \leq E', \\ &= 0 & \text{otherwise} \end{aligned} \quad (C.2)$$

and $\Sigma_{sne}(E' \rightarrow E)$ is a bounded kernel. Repeating the resolvent set discussion for $\kappa \notin C$, Eqs. (2.9)-(2.15), with Eq. (C.1) as the kernel, we find that the complement of C again is the resolvent set for any nonzero ΔE , since both kernels are bounded. However in the limit $\Delta E = 0$ Eq. (C.1) becomes the singular kernel of Eq. (2.25); once more repeating the resolvent set investigation we obtain for Eq. (2.13)

$$\begin{aligned} \phi(E) &= f(E) \frac{1}{2} \Sigma_{se}(E) \phi(E) + f(E) \int_E^{\infty} \frac{1}{2} \Sigma_{sne}(E' \rightarrow E) \phi(E') dE' + \\ &+ g(E). \end{aligned} \quad (C.3)$$

Defining

$$\Lambda_e(E) = 1 - \frac{1}{2} f(E) \Sigma_{se}(E), \quad (C.4)$$

Eq. (C.3) becomes

$$\begin{aligned} \phi(E) &= \frac{f(E)}{\Lambda_e(E)} \int_E^{\infty} \frac{1}{2} \Sigma_{sne}(E' \rightarrow E) \phi(E') dE' + g(E), \\ &\kappa \notin C. \end{aligned} \quad (C.5)$$

For values of κ (entering through $f(E)$) and E such that Λ_e vanishes, Eq. (C.5) will not be invertible and κ will be in the spectrum of the wave Boltzmann operator [32,33]. For a particular E , Eq. (C.4) is the dispersion law function for the point spectrum of the monoenergetic

wave transport equation; as E varies, values of κ which satisfy the dispersion law will sweep out a line, the "elastic continuum" [32,33], in the complex κ plane exterior to the transport continuum C . For a monoenergetic source this additional spectral contribution evidently will give rise to modes which appear to be discrete modes having the source energy, in accordance with the discussion in Chapter II. This appearance of additional spectrum only in the limit $\Delta E = 0$ is not surprising from a mathematical point of view; however, physically it is evident that the role of the elastic spectral contribution must have been assumed for $\Delta E \approx 0$ by superimposed continuum eigenfunctions for $\kappa \in C$. Thus we must be cautious in regarding continuum modes as more attenuated than discrete regular modes, since superimposed continuum modes clearly can exhibit highly persistent spatial behavior.

Another simple limiting process can be employed to model the same phenomenon, making use of the elastic continuum. Define the kernel

$$\Sigma_s(E' \rightarrow E) = \beta \Sigma_s(E') \delta(E' - E) + (1 - \beta) \Sigma_s(E') K(E' \rightarrow E) ,$$

$$0 \leq \beta \leq 1 \tag{C.6}$$

so that β acts like a detector energy window, determining the fraction of neutrons which may be regarded as monoenergetic after one collision. The "elastic continuum" T corresponding to this model is shown schematically in Figure C.1. For a particular energy E_0 the corresponding line in the transport continuum is denoted by $\kappa(E_0)$, while $\kappa_e(E_0)$ is the value of κ which satisfies the elastic dispersion law $\Lambda_e(E_0) = 0$. We note that for this model the apparent attenuation and wave length of

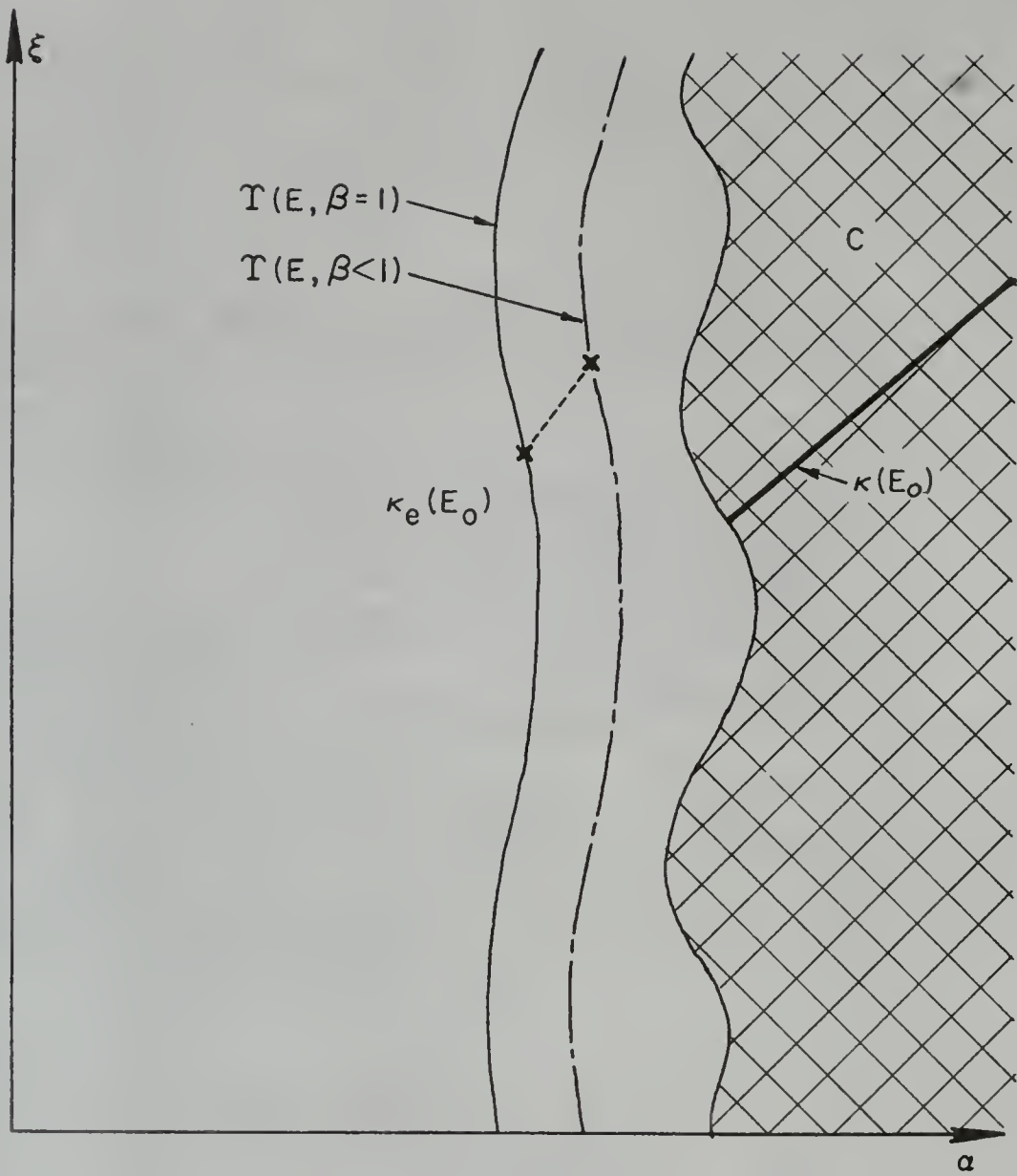


Figure C.1 Schematic diagram of the "elastic continuum" for macroscopically elastic scattering.

the elastic mode depend on the value of β ; this may be seen by using the definition of $f(E)$

$$f(E) = \frac{1}{\kappa} \ln\left(\frac{a+\kappa}{a-\kappa}\right) \quad (C.7)$$

in the elastic dispersion function, Eq. (C.4) so that $\Lambda_e = 0$ may be rearranged to give

$$\begin{aligned} \kappa &= \frac{1}{2} \Sigma_{se} \ln\left(\frac{a+\kappa}{a-\kappa}\right) \\ &= \frac{1}{2} \beta \Sigma_s \ln\left(\frac{a+\kappa}{a-\kappa}\right). \end{aligned} \quad (C.8)$$

For κ_e not too near the continuum, so that variations in the logarithm are slow, κ varies almost linearly with β , as shown in Figure C.1. Evidently, then, the observed modal propagation constants in an experiment would depend on the detector energy window.

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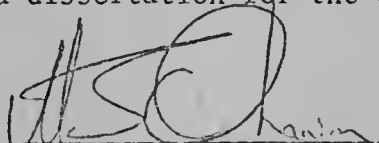
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BIOGRAPHICAL SKETCH

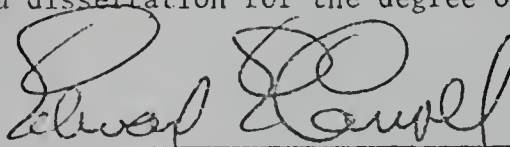
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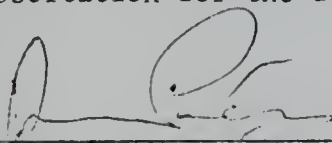
Mihran J. Ohanian
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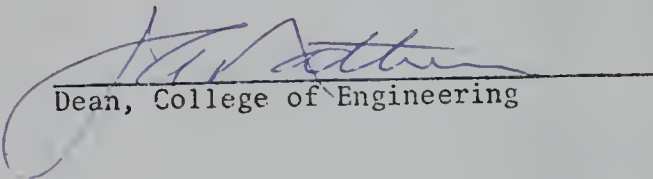
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This dissertation was submitted to the Dean of the College of Engineering and to the Graduate Council, and was accepted as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

June, 1974



Dean, College of Engineering

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